

PMID- 26025550

OWN - NLM

STAT- In-Data-Review

DA - 20150710

IS - 1618-2650 (Electronic)

VI - 407

IP - 19

DP - 2015 Jul

TI - Optimization and comparison of several extraction methods for determining perfluoroalkyl substances in abiotic environmental solid matrices using liquid chromatography-mass spectrometry.

PG - 5767-81

LID - 10.1007/s00216-015-8759-2 [doi]

AB - In this study, four extraction methods of perfluoroalkyl substances (PFASs) in soils and sediments were validated and compared in order to select the one that provides the best recoveries and the highest sensitivity. The determination of PFASs was carried out by liquid chromatography-tandem mass spectrometry. The extraction methods compared were based on (i) an aqueous solution of acetic acid and methanol (recoveries 44-125 %, relative standard deviation (RSD) <25 %), (ii) methanol (34-109 %, <25 %), (iii) sodium hydroxide digestion (24-178 %, <49 %), and (iv) ion pair (35-179 %, <31 %). The best results were obtained with methanol extraction, which recovered a greater number of PFASs and provided values between 45-103 % in sediment and 34-109 % in soil with RSDs <25 % and limits of quantification (LOQs) between 0.02-0.31 and 0.01-6.00 ng g<sup>(-1)</sup>, respectively. The selected method was successfully applied to Segura River sediments and soil samples taken near the Turia River. This study demonstrates the presence of PFASs in the studied rivers of the Valencian Community (0.07-14.91 ng g<sup>(-1)</sup> in Segura River sediments; 0.02-64.04 ng g<sup>(-1)</sup> in Turia River soils). Graphical Abstract  
Selected matrices and extraction methods for determination of perfluoroalkyl substances.

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FAU - Pico, Yolanda

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LA - eng

PT - Journal Article

DEP - 20150530

PL - Germany

TA - Anal Bioanal Chem

JT - Analytical and bioanalytical chemistry

JID - 101134327

SB - IM  
EDAT- 2015/05/31 06:00  
MHDA- 2015/05/31 06:00  
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AID - 10.1007/s00216-015-8759-2 [doi]  
PST - ppublish  
SO - Anal Bioanal Chem. 2015 Jul;407(19):5767-81. doi: 10.1007/s00216-015-8759-2. Epub  
2015 May 30.

PMID- 26047527  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150707  
IS - 1520-6882 (Electronic)  
IS - 0003-2700 (Linking)  
VI - 87  
IP - 13  
DP - 2015 Jul 7  
TI - Exploring Fluorous Affinity by Liquid Chromatography.  
PG - 6854-60

LID - 10.1021/acs.analchem.5b01212 [doi]

AB - Terms such as "fluorous affinity" and "fluorophilicity" have been used to describe the unique partition and sorption properties often exhibited by highly fluorinated organic compounds, that is molecules rich in sp(3) carbon-fluorine bonds. In this work, we made use of a highly fluorinated stationary phase and a series of benzene derivatives to study the effect of one single perfluorinated carbon on the chromatographic behavior and adsorption properties of molecules. For this purpose, the adsorption equilibria of alpha,alpha,alpha-trifluorotoluene, toluene, and other alkylbenzenes have been studied by means of nonlinear chromatography in a variety of acetonitrile/water eluents. Our results reveal that one single perfluorinated carbon is already enough to induce a drastic change in the adsorption properties of molecules on the perfluorinated stationary phase. In particular, it has been found that adsorption is monolayer if the perfluoroalkyl carbon is present but that, when this unit is missing, molecules arrange as multilayer stack structures. These findings can contribute to the understanding of molecular mechanisms of fluorous affinity.

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LA - eng

PT - Journal Article

DEP - 20150616

PL - United States

TA - Anal Chem

JT - Analytical chemistry

JID - 0370536

SB - IM

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PHST- 2015/06/16 [aheadofprint]

AID - 10.1021/acs.analchem.5b01212 [doi]

PST - ppublish

SO - Anal Chem. 2015 Jul 7;87(13):6854-60. doi: 10.1021/acs.analchem.5b01212. Epub 2015 Jun 16.

PMID- 26153615

OWN - NLM

STAT- In-Data-Review

DA - 20150804

IS - 1520-6882 (Electronic)

IS - 0003-2700 (Linking)

VI - 87

IP - 15

DP - 2015 Aug 4

TI - Fluorinated Pickering Emulsions with Nonadsorbing Interfaces for Droplet-based Enzymatic Assays.

PG - 7938-43

LID - 10.1021/acs.analchem.5b01753 [doi]

AB - This work describes the use of fluorinated Pickering emulsions with nonadsorbing interfaces in droplet-based enzymatic assays. State-of-the-art droplet assays

have relied on one type of surfactants consisting of perfluorinated polyether and polyethylene glycol (PFPE-PEG). These surfactants are known to have limitations including the tedious synthesis and interdrop molecular transport which leads to the cross-contamination of droplet contents. Previously we have shown that replacing surfactants with nanoparticles as droplet stabilizers mitigate interdrop transport of small molecules. The nonspecific adsorption of enzymes on nanoparticle surface, however, could cause structural changes in enzymes and consequently the loss of enzymatic activity. To overcome such challenge, we render nanoparticle surface nonadsorbing to enzymes by in situ adsorption of polyethylene glycol (PEG) on particle surfaces. We show that enzyme activities are preserved in droplets stabilized by PEG-adsorbed nanoparticles, and are comparable with those in drops stabilized by PFPE-PEG surfactants. In addition, our nonadsorbing Pickering emulsions successfully prevent interdrop molecular transport, thereby maintaining the accuracy of droplet assays. The particles are also simple and economical to synthesize. The PEG-adsorbed nanoparticles described in this work are thus a competitive alternative to the current surfactant system, and can potentially enable new droplet-based biochemical assays.

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LA - eng

PT - Journal Article

DEP - 20150721

PL - United States

TA - Anal Chem

JT - Analytical chemistry

JID - 0370536

SB - IM

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AID - 10.1021/acs.analchem.5b01753 [doi]

PST - ppublish

SO - Anal Chem. 2015 Aug 4;87(15):7938-43. doi: 10.1021/acs.analchem.5b01753. Epub 2015 Jul 21.

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OWN - NLM  
 STAT- Publisher  
 DA - 20150731  
 LR - 20150801  
 IS - 1521-3773 (Electronic)  
 IS - 1433-7851 (Linking)  
 DP - 2015 Jul 29  
 TI - Benzylic C(sp<sup>3</sup>)H Perfluoroalkylation of Six-Membered Heteroaromatic Compounds.  
 LID - 10.1002/anie.201505335 [doi]  
 AB - Successful benzylic C(sp<sup>3</sup>)H trifluoromethylation, pentafluoroethylation, and heptafluoropropylation of six-membered heteroaromatic compounds were achieved as the first examples of a practical benzylic C(sp<sup>3</sup>)H perfluoroalkylation. In these reactions, BF<sub>2</sub> Cn F<sub>2n+1</sub> (n=1-3) functioned as both a Lewis acid to activate the benzylic position and a Cn F<sub>2n+1</sub> (n=1-3) source. The perfluoroalkylation proceeded at both terminal and internal positions of the alkyl chains. Perfluoroalkylated products were obtained in moderate to excellent yields, even on gram scale, and in a sequential procedure without isolation of the intermediates. By using this method, trifluoromethylation of a bioactive compound, as well as introduction of a CF<sub>3</sub> group into a bioactive molecular skeleton, proceeded regioselectively.  
 CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.  
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 LA - ENG  
 PT - JOURNAL ARTICLE  
 DEP - 20150729  
 TA - Angew Chem Int Ed Engl  
 JT - Angewandte Chemie (International ed. in English)  
 JID - 0370543  
 OTO - NOTNLM  
 OT - Lewis acids  
 OT - arenes  
 OT - boranes  
 OT - fluorine

OT - heterocycles  
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AID - 10.1002/anie.201505335 [doi]  
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SO - Angew Chem Int Ed Engl. 2015 Jul 29. doi: 10.1002/anie.201505335.

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OWN - NLM  
STAT- In-Data-Review  
DA - 20150722  
LR - 20150801  
IS - 1521-3773 (Electronic)  
IS - 1433-7851 (Linking)  
VI - 54  
IP - 31  
DP - 2015 Jul 27  
TI - Nickel-Catalyzed Alkyl-Alkyl Cross-Couplings of Fluorinated Secondary Electrophiles: A General Approach to the Synthesis of Compounds having a Perfluoroalkyl Substituent.  
PG - 9047-51  
LID - 10.1002/anie.201503297 [doi]  
AB - Fluorinated organic molecules are of interest in fields ranging from medicinal chemistry to polymer science. Described herein is a mild, convenient, and versatile method for the synthesis of compounds bearing a perfluoroalkyl group attached to a tertiary carbon atom by using an alkyl-alkyl cross-coupling. A nickel catalyst derived from NiCl<sub>2</sub> glyme and a pybox ligand achieves the coupling of a wide range of fluorinated alkyl halides with alkylzinc reagents at room temperature. A broad array of functional groups is compatible with the reaction conditions, and highly selective couplings can be achieved on the basis of differing levels of fluorination. A mechanistic investigation has established that the presence of 2,2,6,6-tetramethyl-1-piperidinyloxy (TEMPO) inhibits cross-coupling under these conditions and that a TEMPO-electrophile adduct can be isolated.  
CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.  
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GR - R01 GM062871/GM/NIGMS NIH HHS/United States

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 DEP - 20150612  
 PL - Germany  
 TA - Angew Chem Int Ed Engl  
 JT - Angewandte Chemie (International ed. in English)  
 JID - 0370543  
 SB - IM  
 PMC - PMC4521909  
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 OID - NLM: PMC4521909 [Available on 07/27/16]  
 OTO - NOTNLM  
 OT - cross-coupling  
 OT - fluorine  
 OT - homogeneous catalysis  
 OT - nickel  
 OT - zinc  
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 AID - 10.1002/anie.201503297 [doi]  
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PMID- 26142120  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150704  
 LR - 20150705  
 IS - 1432-0703 (Electronic)  
 IS - 0090-4341 (Linking)  
 DP - 2015 Jul 4  
 TI - Organohalogen Contaminants and Vitamins in Northern Fur Seals (*Callorhinus ursinus*) Collected During Subsistence Hunts in Alaska.  
 AB - During native subsistence hunts from 1987 to 2007, blubber and liver samples from 50 subadult male northern fur seals (*Callorhinus ursinus*) were collected on St. Paul Island, Alaska. Samples were analyzed for legacy persistent organic pollutants (POPs), recently phased-out/current-use POPs, and vitamins. The legacy POPs measured from blubber samples included polychlorinated biphenyl congeners, DDT (and its metabolites), chlorobenzenes, chlordanes, and mirex. Recently phased-out/current-use POPs included in the blubber analysis were the flame retardants, polybrominated diphenyl ethers, and hexabromocyclododecanes. The chemical surfactants, perfluorinated alkyl acids, and vitamins A and E were

assessed in the liver samples. Overall, concentrations of legacy POPs are similar to levels seen in seal samples from other areas of the North Pacific Ocean and the Bering Sea. Statistically significant correlations were seen between compounds with similar functions (pesticides, flame retardants, vitamins). With sample collection spanning two decades, the temporal trends in the concentrations of POPs and vitamins were assessed. For these animals, the concentrations of the legacy POPs tend to decrease or stay the same with sampling year; however, the concentrations of the current-use POPs increased with sampling year. Vitamin concentrations tended to stay the same across the sampling years. With the population of northern fur seals from St. Paul Island on the decline, a detailed assessment of exposure to contaminants and the correlations with vitamins fills a critical gap for identifying potential population risk factors that might be associated with health effects.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150704

TA - Arch Environ Contam Toxicol

JT - Archives of environmental contamination and toxicology



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AID - 10.1007/s00244-015-0179-y [doi]  
PST - aheadofprint  
SO - Arch Environ Contam Toxicol. 2015 Jul 4.

PMID- 26193847

OWN - NLM

STAT- Publisher

DA - 20150721

LR - 20150722

IS - 1434-3916 (Electronic)

IS - 0936-8051 (Linking)

DP - 2015 Jul 21

TI - Radiologic healing of lateral femoral wall fragments after intramedullary nail fixation for A3.3 intertrochanteric fractures.

AB - INTRODUCTION: Intramedullary nail fixation is a useful treatment option for A3 intertrochanteric fractures. Occasionally, we have encountered displaced lateral femoral wall (LFW) fragment during surgery with intramedullary nail system. We investigated the postoperative spontaneous reduction of displaced LFW fragments without further fixation and the factors that affected the spontaneous reduction of displaced LFW fragments. MATERIALS AND METHODS: Forty-four patients with A3.3 intertrochanteric fracture were treated by surgery using intramedullary nails (PFNA; Synthes, Paoli) between March 2007 and December 2012. All patients had a minimum follow-up period of 12 months. We calculated the amount of spontaneous reduction of the displaced LFW fragments from immediate postoperative and last follow-up anteroposterior radiographs. We measured the tilting angle of the LFW fragment, tip-apex distance (TAD), and telescoping of the blade, and evaluated the quality of postoperative reduction. RESULTS: Twenty-five of the 44 patients had displaced LFW fragments, and the average amount of spontaneous reduction of the displaced LFW fragment was 4.8 mm with statistical significance ( $p = 0.005$ ). The average tilting angle of all patients was  $-4.97$  degrees, telescoping was 6.83 mm, and TAD was 19.77 mm. Twenty-one patients had good quality of reduction, 21 had acceptable quality, and 2 had poor quality. Multivariate logistic regression analysis for these factors indicated that tilting angle was the only significant factor related to spontaneous reduction of a displaced LFW fragment ( $p = 0.007$ , odds ratio = 1.336). CONCLUSIONS: In intramedullary nailing of A3.3 intertrochanteric fractures, the displaced LFW fragments tend to reduce spontaneously without any additional fixation during the postoperative period. We conclude that no additional fixation is needed for the displaced LFW fragment after surgery with intramedullary nail.

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LA - ENG

PT - JOURNAL ARTICLE

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TA - Arch Orthop Trauma Surg

JT - Archives of orthopaedic and trauma surgery

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STAT- In-Process

DA - 20150709

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VI - 15

DP - 2015

TI - A novel device for assessing dark adaptation in field settings.

PG - 74

LID - 10.1186/s12886-015-0062-7 [doi]

AB - BACKGROUND: Aberrant dark adaptation is common to many ocular diseases and pathophysiological conditions, including vitamin A deficiency, cardiopulmonary diseases, and hypoxia. Scotopic vision and pupillary responsiveness have typically been measured using subjective, time-consuming methods. Existing techniques are particularly challenging for use in developing country settings, where vitamin A deficiency remains a major public health problem. Our aim was design a compact, low cost, and easily operated device to assess dark adaptation

in the field. METHODS: The Portable Field Dark Adaptometer (PFDA) incorporates a digital camera, a retinal bleaching flash, and a Ganzfeld light source inside a pair of light-obscuring goggles. After a ~10 min period of dark adaption, the infrared camera digitally records afferent pupillary responses to graded light stimuli (-2.9 to 0.1 log cd/m<sup>2</sup>). We tested this device in a variety of field settings to assess: a) ease of use and b) whether test data could clearly and accurately depict the well-known dose-response relationship between light intensity and pupil contraction. A total of 822 videos were collected. We used an open source video analysis software to measure pupil size in pixel units. Pupillary responsiveness was expressed as the percent change in pupil size from pre- to post-light exposure. Box plots, t test, and multi-level mixed effects linear regression modeling were used to characterize the relationship between light intensity and pupillary response. RESULTS: The PFDA was employed with only minor technical challenges in Bangladesh, Kenya, Zambia, and Peru. Our data show a clear linear increase in pupillary constriction with increasing log light intensity. Light intensity was a strong predictor of pupillary response, regardless of baseline pupil size. CONCLUSIONS: The consistent physiological response demonstrated here supports the use of the PFDA as a reliable tool to measure dark adaptation. As a next step, PFDA measurements will be validated against biochemical indicators of vitamin A status and hypoxemia. Ultimately, this new technology may provide a novel approach for nutritional assessment, with potential clinical applications.

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LA - eng

GR - 5R25TW009340/TW/FIC NIH HHS/United States

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PT - Journal Article

PT - Research Support, N.I.H., Extramural

PT - Research Support, Non-U.S. Gov't

DEP - 20150709

PL - England

TA - BMC Ophthalmol

JT - BMC ophthalmology

JID - 100967802

SB - IM

PMC - PMC4496941

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PMID- 26184495

OWN - NLM

STAT- In-Data-Review

DA - 20150803

LR - 20150804

IS - 1421-9786 (Electronic)

IS - 1015-9770 (Linking)

VI - 40

IP - 1-2

DP - 2015

TI - The RoPE Score and Right-to-Left Shunt Severity by Transcranial Doppler in the CODICIA Study.

PG - 52-8

LID - 10.1159/000430998 [doi]

AB - BACKGROUND: For patients with cryptogenic stroke (CS) and patent foramen ovale (PFO), it is unknown whether the magnitude of right-to-left shunt (RLSh) measured by contrast transcranial Doppler (c-TCD) is correlated with the likelihood an identified PFO is related to CS as determined by the Risk of Paradoxical Embolism (RoPE) score. Additionally, for patients with CS, it is unknown whether PFO assessment by c-TCD is more sensitive for identifying RLSh compared with transesophageal echocardiography (TEE). Our aim was to determine the significance

of RLSh grade by c-TCD in patients with PFO and CS. METHODS: We evaluated patients with CS who had RLSh quantified by c-TCD in the Multicenter Study into RLSh in Cryptogenic Stroke (CODICIA) to determine whether there is an association between c-TCD shunt grade and the RoPE Score. For patients who underwent c-TCD and TEE, we determined whether there is agreement in identifying and grading RLSh between these two modalities. RESULTS: The RoPE score predicted the presence versus the absence of RLSh documented by c-TCD (c-statistic = 0.66). For patients with documented RLSh by c-TCD, shunt severity was correlated with increasing RoPE score (rank correlation ( $r$ ) = 0.15,  $p$  = 0.01). Among 293 patients who had both c-TCD and TEE performed, c-TCD was more sensitive (98.7%) for detecting RLSh. Of the 97 patients with no PFO identified on TEE, 28 (29%) had a large amount of RLSh seen on c-TCD. CONCLUSIONS: For patients with CS, severity of RLSh by c-TCD is positively correlated with the RoPE score, indicating that this technique for shunt grading identifies patients more likely to have pathogenic rather than incidental PFOs. c-TCD is also more sensitive in detecting RLSh than TEE. These findings suggest an important role for c-TCD in the evaluation of PFO in the setting of CS. (c) 2015 S. Karger AG, Basel.

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GR - R01 NS062153/NS/NINDS NIH HHS/United States

GR - R21 NS079826/NS/NINDS NIH HHS/United States

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GR - UL1 TR001064/TR/NCATS NIH HHS/United States

PT - Journal Article

DEP - 20150711

PL - Switzerland

TA - Cerebrovasc Dis

JT - Cerebrovascular diseases (Basel, Switzerland)

JID - 9100851

SB - IM

PMC - PMC4523222

MID - NIHMS697367

OID - NLM: NIHMS697367 [Available on 07/11/16]

OID - NLM: PMC4523222 [Available on 07/11/16]

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MHDA- 2015/07/18 06:00

CRDT- 2015/07/18 06:00  
 PMCR- 2016/07/11 00:00  
 PHST- 2014/12/19 [received]  
 PHST- 2015/04/27 [accepted]  
 PHST- 2015/07/11 [aheadofprint]  
 AID - 000430998 [pii]  
 AID - 10.1159/000430998 [doi]  
 PST - ppublish  
 SO - Cerebrovasc Dis. 2015;40(1-2):52-8. doi: 10.1159/000430998. Epub 2015 Jul 11.  
  
 PMID- 26041689  
 OWN - NLM  
 STAT- PubMed-not-MEDLINE  
 DA - 20150616  
 DCOM- 20150818  
 IS - 1364-548X (Electronic)  
 IS - 1359-7345 (Linking)  
 VI - 51  
 IP - 52  
 DP - 2015 Jul 4  
 TI - Photoinduced reductive perfluoroalkylation of phosphine oxides: synthesis of  
       P-perfluoroalkylated phosphines using TMDPO and perfluoroalkyl iodides.  
 PG - 10385-8  
 LID - 10.1039/c5cc03427b [doi]  
 AB - A photoinduced reaction between TMDPO (diphenyl(2,4,6-trimethylbenzoyl)-phosphine  
       oxide) and perfluoroalkyl iodides successfully affords  
       P-(perfluoroalkyl)diphenylphosphines as promising ligands for recyclable  
       catalysts. Interestingly, the perfluoroalkylation reaction involves the reduction  
       of phosphorus(V) compounds to phosphorus(III) species. The advantages of the  
       present reaction include the use of an air-stable phosphorus source and good  
       yields of P-perfluoroalkylphosphines in short reaction times.  
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 FAU - Kawaguchi, Shin-ichi  
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 FAU - Ogawa, Akiya  
 AU - Ogawa A  
 LA - eng  
 PT - Journal Article  
 PL - England  
 TA - Chem Commun (Camb)  
 JT - Chemical communications (Cambridge, England)  
 JID - 9610838  
 EDAT- 2015/06/05 06:00  
 MHDA- 2015/06/05 06:01

CRDT- 2015/06/05 06:00  
AID - 10.1039/c5cc03427b [doi]  
PST - ppublish  
SO - Chem Commun (Camb). 2015 Jul 4;51(52):10385-8. doi: 10.1039/c5cc03427b.

PMID- 26129829  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150718  
IS - 1521-3765 (Electronic)  
IS - 0947-6539 (Linking)  
VI - 21  
IP - 31  
DP - 2015 Jul 27  
TI - Perfluoroalkyl and -aryl Zinc Ate Complexes: Generation, Reactivity, and Synthetic Application.  
PG - 10993-6  
LID - 10.1002/chem.201501811 [doi]  
AB - A combination of dimethylzinc, perfluoroalkyl iodide, and LiCl afforded a new type of perfluoroalkyl (RF ) zinc ate complex. These complexes show much greater thermal stability than conventional perfluorinated metal species, such as RF -lithium species and Grignard reagents, and they can be used at room temperature or higher. The results of DFT calculations on the origin of the enhanced stability are reported and the synthetic utility of RF -zincate complexes is demonstrated.  
CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.  
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LA - eng

PT - Journal Article

DEP - 20150630

PL - Germany

TA - Chemistry

JT - Chemistry (Weinheim an der Bergstrasse, Germany)

JID - 9513783

SB - IM

OTO - NOTNLM

OT - ate complexes

OT - chemoselectivity

OT - density functional calculations

OT - perfluoroalkylation

OT - zinc

EDAT- 2015/07/02 06:00

MHDA- 2015/07/02 06:00

CRDT- 2015/07/02 06:00

PHST- 2015/05/08 [received]

PHST- 2015/06/30 [aheadofprint]

AID - 10.1002/chem.201501811 [doi]

PST - ppublish

SO - Chemistry. 2015 Jul 27;21(31):10993-6. doi: 10.1002/chem.201501811. Epub 2015 Jun 30.

PMID- 26177718

OWN - NLM

STAT- In-Data-Review

DA - 20150724

IS - 1521-3765 (Electronic)

IS - 0947-6539 (Linking)

VI - 21

IP - 32

DP - 2015 Aug 3

TI - Monitoring Glycan-Protein Interactions by NMR Spectroscopic Analysis: A Simple Chemical Tag That Mimics Natural CH-pi Interactions.



PG - 11408-16

LID - 10.1002/chem.201501248 [doi]

AB - Detection of molecular recognition processes requires robust, specific, and easily implementable sensing methods, especially for screening applications. Here, we propose the difluoroacetamide moiety (an acetamide bioisoster) as a novel tag for detecting by NMR analysis those glycan-protein interactions that involve N-acetylated sugars. Although difluoroacetamide has been used previously as a substituent in medicinal chemistry, here we employ it as a specific sensor to monitor interactions between GlcNAc-containing glycans and a model lectin (wheat germ agglutinin). In contrast to the widely employed trifluoroacetamide group, the difluoroacetamide tag contains geminal (1) H and (19) F atoms that allow both (1) H and (19) F NMR methods for easy and robust detection of molecular recognition processes involving GlcNAc- (or GalNAc-) moieties over a range of binding affinities. The CHF<sub>2</sub> CONH- moiety behaves in a manner that is very similar to that of the natural acetamide fragment in the involved aromatic-sugar interactions, providing analogous binding energy and conformations, whereas the perfluorinated CF<sub>3</sub> CONH- analogue differs more significantly.

CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

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 LA - eng  
 PT - Journal Article  
 DEP - 20150714  
 PL - Germany  
 TA - Chemistry  
 JT - Chemistry (Weinheim an der Bergstrasse, Germany)  
 JID - 9513783  
 SB - IM  
 OTO - NOTNLM  
 OT - NMR spectroscopy  
 OT - fluorine  
 OT - molecular modeling  
 OT - molecular recognition  
 OT - noncovalent interactions  
 EDAT- 2015/07/17 06:00  
 MHDA- 2015/07/17 06:00  
 CRDT- 2015/07/17 06:00  
 PHST- 2015/03/30 [received]  
 PHST- 2015/07/14 [aheadofprint]  
 AID - 10.1002/chem.201501248 [doi]  
 PST - ppublish  
 SO - Chemistry. 2015 Aug 3;21(32):11408-16. doi: 10.1002/chem.201501248. Epub 2015 Jul 14.  
  
 PMID- 26189958  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150818  
 LR - 20150818  
 IS - 1521-3765 (Electronic)  
 IS - 0947-6539 (Linking)  
 VI - 21  
 IP - 35  
 DP - 2015 Aug 24  
 TI - CF Activation in Perfluorinated Arenes with Isonitriles under UV-Light

Irradiation.

PG - 12295-12298

LID - 10.1002/chem.201502298 [doi]

AB - Due to the great value of fluorinated arenes in agrochemistry, medicinal chemistry and materials science, development of methods for preparation of fluorinated arenes is of high importance. They can be either accessed by arene fluorination or by partial arene defluorination. However, the carbonfluorine bond belongs to the strongest sigma-bonds, which renders CF activation highly challenging. Here it is shown that aryl and alkyl isonitriles efficiently activate the strong CF bond in perfluoroarenes by simple UV irradiation under mild conditions. Reactions proceed by formal direct insertion of the isonitrile into the CF bond without any transition metal. Activation occurs at arene CF bonds whereas aliphatic CF bonds remain unreacted. For selected perfluoroarenes CF activation occurs with high regioselectivity and resulting imidoyl fluorides are transformed into other valuable compounds. Theoretical studies give insights into the reaction mechanism.

CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150717

TA - Chemistry

JT - Chemistry (Weinheim an der Bergstrasse, Germany)

JID - 9513783

OTO - NOTNLM

OT - CF activation

OT - fluorine

OT - perfluoroarene

OT - photochemistry

OT - transition-metal free  
 EDAT- 2015/07/21 06:00  
 MHDA- 2015/07/21 06:00  
 CRDT- 2015/07/21 06:00  
 PHST- 2015/06/12 [received]  
 PHST- 2015/07/17 [aheadofprint]  
 AID - 10.1002/chem.201502298 [doi]  
 PST - ppublish  
 SO - Chemistry. 2015 Aug 24;21(35):12295-12298. doi: 10.1002/chem.201502298. Epub 2015 Jul 17.  
  
 PMID- 26178437  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150818  
 LR - 20150818  
 IS - 1521-3765 (Electronic)  
 IS - 0947-6539 (Linking)  
 VI - 21  
 IP - 35  
 DP - 2015 Aug 24  
 TI - Functionalized Pentafluoroethylphosphanes.  
 PG - 12326-12336  
 LID - 10.1002/chem.201501733 [doi]  
 AB - Bis(diethylamino)pentafluoroethylphosphane represents a versatile starting material for the synthesis of functionalized pentafluoroethylphosphanes. Perfluoroalkyl substituted aminophosphanes themselves already exhibit interesting coordination properties and were treated with the catalytically relevant salts PtCl<sub>2</sub> and PdCl<sub>2</sub> affording trans-[Cl<sub>2</sub> M{P(C<sub>2</sub>F<sub>5</sub>)(NEt<sub>2</sub>)<sub>2</sub>}]<sub>2</sub>. The hitherto unknown (C<sub>2</sub>F<sub>5</sub>)PBr<sub>2</sub>, accessible in good yields by treatment of C<sub>2</sub>F<sub>5</sub>P(NEt<sub>2</sub>)<sub>2</sub> with HBr, was smoothly transformed into the corresponding phosphane, C<sub>2</sub>F<sub>5</sub>PH<sub>2</sub>, or fluoro derivative, C<sub>2</sub>F<sub>5</sub>PF<sub>2</sub>. Acidic hydrolysis of C<sub>2</sub>F<sub>5</sub>P(NEt<sub>2</sub>)<sub>2</sub> yielded the phosphinic acid C<sub>2</sub>F<sub>5</sub>P(O)(OH)H, the anion of which was structurally characterized. The phosphinic acid smoothly adds to the carbonyl group of acetone under PC bond formation. An analogous reaction with aldehydes, for example, salicyl aldehyde, offers the possibility to generate stereocenters.  
 CI - (c) 2015 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.  
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 LA - ENG  
 PT - JOURNAL ARTICLE  
 DEP - 20150714  
 TA - Chemistry  
 JT - Chemistry (Weinheim an der Bergstrasse, Germany)  
 JID - 9513783  
 OTO - NOTNLM  
 OT - fluorine  
 OT - functionalization  
 OT - phosphinic acid  
 OT - phosphorus  
 OT - transition metals  
 EDAT- 2015/07/17 06:00  
 MHDA- 2015/07/17 06:00  
 CRDT- 2015/07/17 06:00  
 PHST- 2015/05/04 [received]  
 PHST- 2015/07/14 [aheadofprint]  
 AID - 10.1002/chem.201501733 [doi]  
 PST - ppublish  
 SO - Chemistry. 2015 Aug 24;21(35):12326-12336. doi: 10.1002/chem.201501733. Epub 2015  
 Jul 14.  
  
 PMID- 26190176  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150720  
 LR - 20150721  
 IS - 1860-7187 (Electronic)  
 IS - 1860-7179 (Linking)  
 DP - 2015 Jul 14  
 TI - Anticancer Organometallic Osmium(II)-p-cymene Complexes.  
 LID - 10.1002/cmdc.201500221 [doi]  
 AB - Osmium compounds are attracting increasing attention as potential anticancer  
 drugs. In this context, a series of bifunctional organometallic  
 osmium(II)-p-cymene complexes functionalized with alkyl or perfluoroalkyl groups  
 were prepared and screened for their antiproliferative activity. Three compounds  
 from the series display selectivity toward cancer cells, with moderate  
 cytotoxicity observed against human ovarian carcinoma (A2780) cells, whereas no  
 cytotoxicity was observed on non-cancerous human embryonic kidney (HEK-293) cells

and human endothelial (ECRF24) cells. Two of these three cancer-cell-selective compounds induce cell death largely via apoptosis and were also found to disrupt vascularization in the chicken embryo chorioallantoic membrane (CAM) model. Based on these promising properties, these compounds have potential clinical applications.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150714

TA - ChemMedChem

JT - ChemMedChem

JID - 101259013

OTO - NOTNLM

OT - antitumor agents

OT - bioorganometallic chemistry

OT - chorioallantoic membrane model

OT - osmium complexes

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AID - 10.1002/cmdc.201500221 [doi]

PST - aheadofprint

SO - ChemMedChem. 2015 Jul 14. doi: 10.1002/cmdc.201500221.

PMID- 26203866

OWN - NLM

STAT- Publisher

DA - 20150723

LR - 20150724

IS - 1879-1298 (Electronic)

IS - 0045-6535 (Linking)

VI - 138

DP - 2015 Jul 20

TI - Perfluorinated compounds (PFCs) in the atmosphere of Shenzhen, China: Spatial distribution, sources and health risk assessment.

PG - 511-518

LID - S0045-6535(15)00732-8 [pii]

LID - 10.1016/j.chemosphere.2015.07.012 [doi]

AB - This study investigated the occurrence of perfluorinated compounds (PFCs) in the atmosphere of Shenzhen, China. 11 PFCs, including two perfluoroalkyl sulfonic acids (PFSA, C6 and C8) and perfluoroalkyl carboxylic acids (PFCA, C4-12) were determined by high performance liquid chromatography-negative electrospray ionization-tandem mass spectrometry (HPLC/ESI-MS/MS). Total PFC concentrations ( summation operator PFCs) in the atmospheric samples ranged from 3.4 to 34pgm-3 with an average of 15pgm-3. Perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) were the two most abundant PFCs and on average accounted for 35% and 22% of summation operator PFCs, respectively. summation operator PFCs and total PFCA concentrations ( summation operator PFCA) showed a tendency of low-lying East West, while the distribution of total PFSA concentrations ( summation operator PFSA) was uniform. Higher concentrations of summation operator PFCs were found in Bao'an District which had very well-developed manufacturing industries. PCA model was employed to quantitatively calculate the contributions of sources. The results showed that PFOA-factor, long chain PFCs-factor and PFOS-factor were the three main source categories for PFCs in the atmosphere. Meanwhile, long-distance transport of pollutants from southeastern coastal areas might be another source of PFCs in Shenzhen atmosphere. PFCs in the atmosphere were more positively correlated with the levels PM10 than PM2.5, which indicated PFCs were more likely to adhere to particles with relatively large sizes. The hazard ratios of noncancer risk through breathing based on PFOS and PFOA concentrations were calculated and were less than unity, suggesting that PFCs concentrations may pose no or immediate threat to the residents in Shenzhen.

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LA - ENG  
PT - JOURNAL ARTICLE  
DEP - 20150720  
TA - Chemosphere  
JT - Chemosphere  
JID - 0320657  
OTO - NOTNLM  
OT - Environmental health risk assessment  
OT - Perfluorinated compounds (PFCs)  
OT - Source appointment  
OT - Spatial distribution  
EDAT- 2015/07/24 06:00  
MHDA- 2015/07/24 06:00  
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PHST- 2015/03/04 [received]  
PHST- 2015/06/07 [revised]  
PHST- 2015/07/07 [accepted]



AID - S0045-6535(15)00732-8 [pii]  
 AID - 10.1016/j.chemosphere.2015.07.012 [doi]  
 PST - aheadofprint  
 SO - Chemosphere. 2015 Jul 20;138:511-518. doi: 10.1016/j.chemosphere.2015.07.012.

PMID- 26172515  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150714  
 LR - 20150715  
 IS - 1879-1298 (Electronic)  
 IS - 0045-6535 (Linking)  
 VI - 141  
 DP - 2015 Jul 11  
 TI - Electro-oxidation of perfluorooctanoic acid by carbon nanotube sponge anode and the mechanism.  
 PG - 120-126  
 LID - S0045-6535(15)00716-X [pii]  
 LID - 10.1016/j.chemosphere.2015.06.095 [doi]

AB - As an emerging persistent organic pollutant (POPs), perfluorooctanoic acid (PFOA) exists widely in natural environment. It is of particular significance to develop efficient techniques to remove low-concentration PFOA from the contaminated waters. In this work, we adopted a new material, carbon nanotube (CNT) sponge, as electrode to enhance electro-oxidation and achieve high removal efficiency of low-concentration (100µg/L) PFOA from water. CNT sponge was pretreated by mixed acids to improve the surface morphology, hydrophilicity and the content of carbonyl groups on the surface. The highest removal efficiencies for low-concentration PFOA electrolyzed by acid-treated CNT sponge anode proved higher than 90%. The electro-oxidation mechanism of PFOA on CNT sponge anode was also discussed. PFOA is adsorbed on the CNT sponge rapidly increasing the concentration of PFOA on anode surface. When the potential on the anode is adjusted to more than 3.5V, the adsorbed PFOA undergoes electrochemically oxidation and hydrolysis to produce shorter-chain perfluorocarboxylic acids with less CF<sub>2</sub> unit. The efficient electro-oxidation of PFOA by CNT sponge anode is due to the combined effect of adsorption and electrochemical oxidation. These findings provide an efficient method to remove actual concentration PFOA from water.

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LA - ENG  
PT - JOURNAL ARTICLE  
DEP - 20150711  
TA - Chemosphere  
JT - Chemosphere  
JID - 0320657  
OTO - NOTNLM  
OT - Adsorption  
OT - Carbon nanotube sponge  
OT - Electro-oxidation  
OT - Perfluorooctanoic acid (PFOA)  
EDAT- 2015/07/15 06:00  
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PHST- 2015/05/04 [received]  
PHST- 2015/06/24 [revised]  
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AID - S0045-6535(15)00716-X [pii]  
AID - 10.1016/j.chemosphere.2015.06.095 [doi]  
PST - aheadofprint  
SO - Chemosphere. 2015 Jul 11;141:120-126. doi: 10.1016/j.chemosphere.2015.06.095.  
  
PMID- 25841073  
OWN - NLM  
STAT- In-Process  
DA - 20150429  
IS - 1879-1298 (Electronic)  
IS - 0045-6535 (Linking)  
VI - 131  
DP - 2015 Jul  
TI - Influence of cations on the partition behavior of perfluoroheptanoate (PFHpA) and perfluorohexanesulfonate (PFHxS) on wastewater sludge.  
PG - 178-83

LID - 10.1016/j.chemosphere.2015.03.024 [doi]

LID - S0045-6535(15)00234-9 [pii]

AB - The effects of different cations on the sorption behavior of PFHpA and PFHxS on two types of sludge were investigated in this study. The sodium and potassium ions did not significantly affect PFHpA and PFHxS sorption on different sludge. For calcium and magnesium, the sorption amount of PFAS increased with calcium and magnesium concentration increasing from 1 to 30 mM and then decreased with those increasing from 30 to 100 mM. The sorption level of PFHxS or PFHpA greatly increased with increasing  $Al^{3+}$  and  $Fe^{3+}$  cation concentrations due to the strong sorption and coagulation effects by the formation of aluminum hydroxide (or ferric hydroxide) colloids or precipitates. After the organics in sludge has been removed by thermal treatment, the PFAS sorption on sludge was greatly reduced. Such finding indicated that sorption to organic matter is more important for anionic PFASs than adsorption to mineral surfaces. However, due to the higher content of biological organics, a secondary activated sludge has higher affinity toward PFAS species than chemically enhanced primary treatment sludge. It indicated that the organic types in sludge were also crucial to the sorption levels of PFASs by sludge.

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LA - eng

PT - Journal Article

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JT - Chemosphere

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OT - Cation

OT - PFHpA

OT - PFHxS  
 OT - Partition  
 OT - Sludge  
 OT - Sorption  
 EDAT- 2015/04/05 06:00  
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 AID - S0045-6535(15)00234-9 [pii]  
 AID - 10.1016/j.chemosphere.2015.03.024 [doi]  
 PST - ppublish  
 SO - Chemosphere. 2015 Jul;131:178-83. doi: 10.1016/j.chemosphere.2015.03.024. Epub 2015 Apr 1.  
  
 PMID- 26183570  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150717  
 LR - 20150718  
 IS - 1520-636X (Electronic)  
 IS - 0899-0042 (Linking)  
 DP - 2015 Jul 15  
 TI - Chiroptical Studies on Supramolecular Chirality of Molecular Aggregates.  
 LID - 10.1002/chir.22482 [doi]  
 AB - The attempts of applying chiroptical spectroscopy to supramolecular chirality are reviewed with a focus on vibrational circular dichroism (VCD). Examples were taken from gels, solids, and monolayers formed by low-molecular mass weight chiral gelators. Particular attention was paid to a group of gelators with perfluoroalkyl chains. The effects of the helical conformation of the perfluoroalkyl chains on the formation of chiral architectures are reported. It is described how the conformation of a chiral gelator was determined by comparing the experimental and theoretical VCD spectra together with a model proposed for the molecular aggregation in fibrils. The results demonstrate the potential utility of the chiroptical method in analyzing organized chiral aggregates. Chirality 00:000-000, 2015. (c) 2015 Wiley Periodicals, Inc.  
 CI - (c) 2015 Wiley Periodicals, Inc.  
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 DEP - 20150715  
 TA - Chirality  
 JT - Chirality  
 JID - 8914261  
 OTO - NOTNLM  
 OT - chiral gelator  
 OT - perfluoroalkyl  
 OT - sol-gel transformation  
 OT - supramolecular  
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 PHST- 2015/01/29 [received]  
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 AID - 10.1002/chir.22482 [doi]  
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PMID- 26158776  
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 DA - 20150709  
 LR - 20150715  
 IS - 1477-9234 (Electronic)  
 IS - 1477-9226 (Linking)  
 DP - 2015 Jul 9  
 TI - A (pentafluoroethyl)(trifluoromethyl)carbene complex of iridium and reductive activation of its  $\alpha$ ,  $\beta$ , and  $\gamma$  carbon-fluorine bonds to give perfluoro-2-butyne, perfluoro-1,2,3-butatriene and perfluoro-1-irida-2-methyl-2-cyclobutene) complexes.

AB - The (pentafluoroethyl)(trifluoromethyl)carbene complex  $\text{Cp}^*\text{Ir}(\text{CO})[[\text{double bond, length as m-dash}]\text{C}(\text{CF}_3)(\text{C}_2\text{F}_5)]$  was synthesized by the reductive activation of the  $\alpha$ -C-F bond in the perfluoro-sec-butyl-iridium complex  $\text{Cp}^*\text{Ir}(\text{CO})[\text{CF}(\text{CF}_3)(\text{C}_2\text{F}_5)](\text{I})$  with Na/Pb alloy. This compound exists as two geometric isomers in solution; the structure of one isomer has been determined by a single crystal X-ray diffraction study and contains two independent molecules in the asymmetric unit. Further reduction of this carbene complex with Na/Pb alloy afforded the perfluoro-2-butyne iridium complex  $\text{Cp}^*\text{Ir}(\text{CO})(\eta^2\text{-CF}_3\text{C}[\text{triple bond, length as m-dash}]\text{CCF}_3)$  by an overall 2-electron reduction and elimination of two  $\beta$ -fluorides. When magnesium graphite was utilized as the reducing agent for the further reduction,  $\text{Cp}^*\text{Ir}(\text{CO})(\eta^2\text{-CF}_3\text{C}[\text{triple bond, length as m-dash}]\text{CCF}_3)$  was produced as a minor product and the major product was the perfluoroiridacyclobutene complex  $\text{Cp}^*\text{Ir}(\text{CO})(\eta^2,4\text{-CF}_3\text{CCF}_2)$  resulting from a  $\gamma$ -C-F bond activation. Direct reduction of the precursor

Cp\*Ir(CO)[CF(CF3)(C2F5)](i) with magnesium graphite generated the tetrafluorobutatriene iridium complex Cp\*Ir(CO)(eta2,3-CF2[double bond, length as m-dash]C[double bond, length as m-dash]C[double bond, length as m-dash]CF2) along with the perfluoro-2-butyne complex and perfluoroiridacyclobutene complexes in a ratio of 1 : 2 : 6. These reductive inner-sphere pathways to unsaturated fluorocarbon ligands illustrate that carbon-fluorine bond activation can take place at alpha-, beta- and gamma-carbons but that selectivity in these heterogeneous reductions is difficult to control, with a variety of fluoride eliminations possible for complex perfluoroalkyl ligands. Density Functional Theory (DFT/B3LYP-D3/LACV3P\*\*++) is used to explore the relative energetics of products and intermediates in these reactions.

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LA - ENG

PT - JOURNAL ARTICLE

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DP - 2015 Jul 27

TI - Synthesis, structure, and reactivity of iridium perfluorocarbene complexes: regio- and stereo-specific addition of HCl across a metal carbon double bond.

AB - Reductive activation of an alpha-fluorine in the perfluoroalkyl complexes Cp\*(L)(i)Ir-CF2RF using Mg/graphite leads to perfluorocarbene complexes Cp\*(L)Ir[double bond, length as m-dash]CFRF (L = CO, PMe3; RF = CF3, C2F5, C6F5). New complexes E-Cp\*(PMe3)Ir[double bond, length as m-dash]CFC2F5 and E-Cp\*(CO)Ir[double bond, length as m-dash]CFC6F5 have been characterized by single crystal X-ray diffraction studies, and a comparison of metric parameters

with previously reported analogues is reported. Experimental NMR and computational DFT (B3LYP/LACV3P\*\*++) studies agree that for Ir[double bond, length as m-dash]CFRF complexes (RF = CF<sub>3</sub>, CF<sub>2</sub>CF<sub>3</sub>) the thermodynamic preference for the E or Z isomer depends on the steric requirements of ligand L; when L = CO the Z-isomer (F cis to Cp\*) is preferred and for L = PMe<sub>3</sub> the E-isomer is preferred. When reduction of the precursors is carried out in the dark the reaction is completely selective to produce E- or Z-isomers. Exposure of solutions of these compounds to ambient light results in slow conversion to a photostationary non-equilibrium mixture of E and Z isomers. In the dark, these E/Z mixtures convert thermally to their preferred E or Z equilibrium geometries in an even slower reaction. A study of the temperature dependent kinetics of this dark transformation allows  $\Delta G_{\text{double dagger}}^{298}$  for rotation about the Ir[double bond, length as m-dash]CFCF<sub>3</sub> double bond to be experimentally determined as 25 kcal mol<sup>-1</sup>; a DFT/B3LYP/LACV3P\*\*++ calculation of this rotation barrier is in excellent agreement (27 kcal mol<sup>-1</sup>) with the experimental value. Reaction of HCl with toluene solutions of Cp\*(L)Ir[double bond, length as m-dash]CFRF (L = CO, PMe<sub>3</sub>) or Cp\*(CO)Ir[double bond, length as m-dash]C(CF<sub>3</sub>)<sub>2</sub> at low temperature resulted in regiospecific addition of HCl across the metal carbon double bond, ultimately yielding Cp\*(L)Ir(CHFRF)Cl and Cp\*(CO)Ir[CH(CF<sub>3</sub>)<sub>2</sub>]Cl. Reaction of HCl with single E or Z diastereomers of Cp\*(L)Ir[double bond, length as m-dash]CFRF gives stereospecific cis-addition to give single diastereomers of Cp\*Ir(L)(CHFRF)Cl; addition of HCl to several different E/Z ratios of Cp\*(L)Ir[double bond, length as m-dash]CFRF affords ratios of diastereomeric products Cp\*(L)Ir(CHFRF)Cl identical to the original ratio of starting material isomers. The addition of HCl is therefore demonstrated to be unambiguously regio- and stereo-specific. The observed product regiochemistry of addition of HCl to Ir[double bond, length as m-dash]CF<sub>2</sub>, Ir[double bond, length as m-dash]CFRF, and Ir[double bond, length as m-dash]C(CF<sub>3</sub>)<sub>2</sub> ligands is the same and is not dependent on the ground state energy preference (singlet or triplet) for the free perfluorocarbene. DFT calculations on model HCl addition reactions indicate that this regiochemistry is strongly preferred thermodynamically, but predict that in H $\delta$ +Cl $\delta$ - addition to Cp(PH<sub>3</sub>)Ir[double bond, length as m-dash]CF<sub>2</sub>, H $\delta$ + attack at Ir has a lower energy transition state, while for Cp(PH<sub>3</sub>)Ir[double bond, length as m-dash]CFCF<sub>3</sub> and Cp(PH<sub>3</sub>)Ir[double bond, length as m-dash]C(CF<sub>3</sub>)<sub>2</sub>, H $\delta$ + attack at C is the kinetically preferred pathway. The carbene carbon atoms in Ir[double bond, length as m-dash]CFCF<sub>3</sub> and Ir[double bond, length as m-dash]C(CF<sub>3</sub>)<sub>2</sub> complexes are unambiguously basic towards HCl, while in the Ir[double bond, length as m-dash]CF<sub>2</sub> analogues the carbene carbon is less basic than its Ir partner, and the eventual regiochemistry of HCl addition arises from thermodynamic control.

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FAU - Hughes, Russell P  
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 LA - ENG  
 PT - JOURNAL ARTICLE  
 DEP - 20150727  
 TA - Dalton Trans  
 JT - Dalton transactions (Cambridge, England : 2003)  
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 AID - 10.1039/c5dt02275d [doi]  
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 PMID- 26172122  
 OWN - NLM  
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 DA - 20150714  
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 IS - 1477-9234 (Electronic)  
 IS - 1477-9226 (Linking)  
 DP - 2015 Jul 14  
 TI - Polyfluorinated carba-closo-dodecaboranes with amino and ammonio substituents bonded to boron.  
 AB - The inner salts x-H3N-closo-1-CB11H11 (x = 12, 2) and 7-H3N-12-F-closo-1-CB11H11 were fluorinated with elemental fluorine in anhydrous hydrogen fluoride to give the B-perfluorinated ammonio derivatives 1-H-x-H3N-closo-1-CB11F10 (x = 12, 7, 2). Deprotonation of the ammonio group yielded the corresponding amino-functionalized anions [1-H-x-H2N-closo-1-CB11F10]- (x = 12, 7, 2) that were isolated as [Et4N]+ salts. Hydrolysis of the highly fluorinated inner salts 1-H-x-H3N-closo-1-CB11F10 (x = 12, 7, 2) is very slow in acidic aqueous solutions. This stability of the ammonio derivatives is unprecedented because the related fluorinated anion [1-H2N-closo-1-CB11F11]- is immediately hydrolyzed to simple boron species in the presence of aqueous acids. The ammonio derivatives 1-H-x-H3N-closo-1-CB11F10 (x = 12, 7, 2) are much more acidic compared to their non-fluorinated counterparts as assessed from potentiometric titrations and DFT calculations. The inner salts and the anions were characterized by NMR and vibrational spectroscopy. Solid-state structures of 1-H-12-H3N-closo-1-CB11F10.H2O, 1-H-7-H3N-closo-1-CB11F10.diglyme, 1-H-2-H3N-closo-1-CB11F10.0.5H2O, 7-H3N-12-F-closo-1-CB11H10.(CH3)2CO and [Et4N][1-H-12-H2N-closo-1-CB11F10] were determined by single-crystal X-ray diffraction.  
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 AU - Finze M  
 LA - ENG  
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 DEP - 20150714  
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 JID - 101176026  
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 PMID- 26169553  
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 DA - 20150728  
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 IS - 1477-9234 (Electronic)  
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 DP - 2015 Jul 14  
 TI - Gold trifluoromethyl complexes.  
 AB - This article reviews the synthesis, reactivity and applications of gold trifluoromethyl complexes, which are the only isolated perfluoroalkyl complexes of gold. The most reported examples are neutral Au(i) complexes of the type [Au(CF<sub>3</sub>)L], whereas only two Au(ii) trifluoromethyl complexes have been reported, both being diamagnetic and containing a strong Au-Au bond. A number of Au(iii) trifluoromethyl complexes have been prepared by oxidative addition of halogens or iodotrifluoromethane to Au(i) complexes or, in a few cases, by transmetallation reactions. Owing to the limitations of the available synthetic methods, a lower number of examples is known, particularly for the oxidation states (ii) and (iii). Gold trifluoromethyl complexes present singular characteristics, such as thermal stability, strong Au-C bonds and, in some cases, reactive alpha-C-F bonds. Some of the Au(iii) complexes reported, show unusually easy reductive elimination reactions of trifluoromethylated products which could be applied in the development of gold-catalyzed processes for the trifluoromethylation of organic compounds.  
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 PT - JOURNAL ARTICLE  
 DEP - 20150714  
 TA - Dalton Trans  
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 JID - 101176026  
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 SO - Dalton Trans. 2015 Jul 14.  
  
 PMID- 26143169  
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 DA - 20150722  
 IS - 1090-2414 (Electronic)  
 IS - 0147-6513 (Linking)  
 VI - 120  
 DP - 2015 Oct  
 TI - Determination of perfluorinated sulfonate and perfluorinated acids in tissues of free-living European beaver (castor fiber L.) by d-SPE/ micro-UHPLC-MS/MS.  
 PG - 436-44  
 LID - 10.1016/j.ecoenv.2015.06.029 [doi]  
 LID - S0147-6513(15)00314-0 [pii]  
 AB - Perfluorooctanesulfonate (PFOS) and perfluorooctanoic acid (PFOA) are the main representatives of an rising class of persistent organic pollutants (POPs), perfluorochemicals (PFCs). In this study, determination of selected PFCs concentration in liver, brain, tail, adipose and peritoneum tissues of free-living European beaver (Castor fiber L.) was addressed. Tissue samples, collected from beavers living in Masurian Lakeland (NE Poland), were analyzed by dispersive Solid Phase Extraction (d-SPE) with micro-UHPLC-MS/MS system. In a group of ten selected pefrluorinated compounds only two perfluorinated acids (PFOA and PFNA) and one perfluorinated sulfonate (PFOS) were quantified. PFOA was detected in all analysed tissue samples in both female and male beavers in a range from 0.55 to 0.98ngg(-1) ww whereas PFOS was identified in all analyzed female beaver tissues and only in liver, subcutaneous adipose and peritoneum tissues of male beavers at the concentration level from 0.86 to 5.08ngg(-1) ww. PFNA was only identified in female beaver tissues (liver, subcutaneous adipose and peritoneum) in a range from 1.50 to 6.61ngg(-1) ww. This study demonstrated the bioaccumulation of PFCs in tissue samples collected from beavers living in area known as green lungs of Poland. The results provided in this study indicate for the increasing risk of PFCs occurrence in the environment and the level of PFCs in tissue of free-living European beavers may serve as bioindicator of environmental pollution by these compounds.

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 LA - eng  
 PT - Journal Article  
 DEP - 20150702  
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 TA - Ecotoxicol Environ Saf  
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 JID - 7805381  
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 OTO - NOTNLM  
 OT - Beaver  
 OT - PFCs  
 OT - PFOA  
 OT - PFOS  
 OT - d-SPE  
 OT - micro-UHPLC-MS/MS  
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 AID - S0147-6513(15)00314-0 [pii]  
 AID - 10.1016/j.ecoenv.2015.06.029 [doi]  
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 PMID- 26148742  
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IS - 1476-069X (Electronic)  
IS - 1476-069X (Linking)  
VI - 14  
DP - 2015  
TI - Perfluoroalkyl acids and time to pregnancy revisited: An update from the Danish National Birth Cohort.  
PG - 59  
LID - 10.1186/s12940-015-0040-9 [doi]  
AB - BACKGROUND: We previously demonstrated an association between plasma perfluorooctane sulfonate (PFOS) and perfluorooctanoate (PFOA) and longer time to pregnancy (TTP) in a sample from the Danish National Birth Cohort (DNBC, 1996-2002). In this study we investigated this association in a new sample from the same cohort. METHODS: Sample 1 consisted of 440 women, and Sample 2 consisted of 1161 women from whom we previously published the associations between PFOS or PFOA and TTP. We performed sample-specific and pooled analyses using discrete-time survival analyses to estimate fecundability ratios according to PFOS and PFOA quartiles, adjusted for potential confounders chosen guided by a directed acyclic graph. We also estimated odds ratios for infertility (TTP > 12 months or infertility treatment) according to PFOS and PFOA by multivariable logistic regression. RESULTS: In Sample 1 PFOS was not associated with lower fecundability ratios or infertility, and there was a tendency towards longer TTP with increasing PFOA only in parous women. In Sample 2 previously reported associations were again seen. In the pooled analyses including both parous and nulliparous women fecundability ratios were 13-22 % lower for the three higher quartiles of PFOS or PFOA compared to the reference quartile. CONCLUSIONS: The pooled analyses were driven by the larger old sample, but we did not corroborate our previous finding of an association between high PFOS and longer TTP in the new sample. The tendency towards an association for PFOA and TTP in parous women may be due to reverse causation. Results from the new sample are more in line with the recent literature.  
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 LA - eng  
 PT - Journal Article  
 PT - Research Support, Non-U.S. Gov't  
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 PL - England  
 TA - Environ Health  
 JT - Environmental health : a global access science source  
 JID - 101147645  
 SB - IM  
 PMC - PMC4493954  
 OID - NLM: PMC4493954  
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 AID - 10.1186/s12940-015-0040-9 [doi]  
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 PST - epubliish  
 SO - Environ Health. 2015 Jul 7;14:59. doi: 10.1186/s12940-015-0040-9.  
  
 PMID- 26159541  
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 STAT- In-Process  
 DA - 20150710  
 IS - 1476-069X (Electronic)  
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 VI - 14

DP - 2015

TI - Within- and between-group regression for improving the robustness of causal claims in cross-sectional analysis.

PG - 60

LID - 10.1186/s12940-015-0047-2 [doi]

AB - BACKGROUND: A major objective of environmental epidemiology is to elucidate exposure-health outcome associations. To increase the variance of observed exposure concentrations, researchers recruit individuals from different geographic areas. The common analytical approach uses multilevel analysis to estimate individual-level associations adjusted for individual and area covariates. However, in cross-sectional data this approach does not differentiate between residual confounding at the individual level and at the area level. An approach allowing researchers to distinguish between within-group effects and between-group effects would improve the robustness of causal claims. METHODS: We applied an extended multilevel approach to a large cross-sectional study aimed to elucidate the hypothesized link between drinking water pollution from perfluorooctanoic acid (PFOA) and plasma levels of C-reactive protein (CRP) or lymphocyte counts. Using within- and between-group regression of the individual PFOA serum concentrations, we partitioned the total effect into a within- and between-group effect by including the aggregated group average of the individual exposure concentrations as an additional predictor variable. RESULTS: For both biomarkers, we observed a strong overall association with PFOA blood levels. However, for lymphocyte counts the extended multilevel approach revealed the absence of a between-group effect, suggesting that most of the observed total effect was due to individual level confounding. In contrast, for CRP we found consistent between- and within-group effects, which corroborates the causal claim for the association between PFOA blood levels and CRP. CONCLUSION: Between- and within-group regression modelling augments cross-sectional analysis of epidemiological data by supporting the unmasking of non-causal associations arising from hidden confounding at different levels. In the application example presented in this paper, the approach suggested individual confounding as a probable explanation for the first observed association and strengthened the robustness of the causal claim for the second one.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

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PL - England

TA - Environ Health

JT - Environmental health : a global access science source

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SO - Environ Health. 2015 Jul 10;14:60. doi: 10.1186/s12940-015-0047-2.

PMID- 26159671

OWN - NLM

STAT- Publisher

DA - 20150710

LR - 20150715

IS - 1873-6750 (Electronic)

IS - 0160-4120 (Linking)

VI - 83

DP - 2015 Jul 6

TI - Perfluoroalkyl substances measured in breast milk and child neuropsychological  
development in a Norwegian birth cohort study.

PG - 176-182

LID - S0160-4120(15)30004-0 [pii]

LID - 10.1016/j.envint.2015.06.013 [doi]

AB - Perfluoroalkyl substances (PFASs) are chemicals with potential neurotoxic effects  
although the current evidence is still limited. This study investigated the  
association between perinatal exposure to perfluorooctanesulfonic acid (PFOS) and  
perfluorooctanoic acid (PFOA) and neuropsychological development assessed at 6,  
12 and 24months. We measured PFOS and PFOA in breast milk samples collected one

month after delivery by mothers of children participating in the HUMIS study (Norway). Cognitive and psychomotor development was measured at 6 and at 24months using the Ages and Stages Questionnaire (ASQ-II). Behavioral development was assessed using the infant-toddler symptom checklist (ITSC) at 12 and at 24months. Weighted logistic regression and weighted negative binomial regression models were applied to analyze the associations between PFASs and ASQ-II and ITSC, respectively. The median concentration of PFOS was 110ng/L, while the median for PFOA was 40ng/L. We did not detect an increased risk of having an abnormal score in ASQ-II at 6months or 24months. Moreover, no consistent increase in behavioral problems assessed at 12 and 24months by ITSC questionnaire was detected. We observed no association between perinatal PFOS and PFOA exposure and early neuropsychological development. Further longitudinal studies are needed to confirm the effects of these compounds on neuropsychological development in older children.

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 PT - JOURNAL ARTICLE  
 DEP - 20150706  
 TA - Environ Int  
 JT - Environment international  
 JID - 7807270  
 OTO - NOTNLM  
 OT - Child development  
 OT - Epidemiology  
 OT - Nervous system  
 OT - Neuropsychology  
 OT - Perfluorooctane sulfonic acid  
 OT - Perfluorooctanoic acid  
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 AID - S0160-4120(15)30004-0 [pii]  
 AID - 10.1016/j.envint.2015.06.013 [doi]  
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 PMID- 26232143  
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 DA - 20150801  
 LR - 20150802  
 IS - 1873-6750 (Electronic)  
 IS - 0160-4120 (Linking)  
 VI - 84  
 DP - 2015 Jul 28  
 TI - Perfluoroalkyl acid (PFAA) levels and profiles in breast milk, maternal and cord serum of French women and their newborns.  
 PG - 71-81  
 LID - S0160-4120(15)30020-9 [pii]  
 LID - 10.1016/j.envint.2015.07.014 [doi]  
 AB - One major concern regarding perfluoroalkyl acids (PFAAs) is their potential role in onset of health troubles consecutive to early exposure during the perinatal

period. In the present work, the internal exposure levels of 18 targeted PFAAs were determined in ca. 100 mother-newborn pairs recruited in France between 2010 and 2013. In serum, the cumulated concentrations of the 7 most frequently detected compounds were 5.70ng/mL and 2.83ng/mL (median values) in maternal and cord serum, respectively. Perfluorooctanesulfonic acid (PFOS), perfluorooctanoic acid (PFOA), perfluorohexylesulfonic acid (PFHxS) and perfluorononanoic acid (PFNA) contributed to around 90% of the total PFAAs contamination, with concentration levels and contamination profiles in accordance with other published work in Europe. Levels measured in breast milk were far lower (20 to 150 fold) than those determined in serum. Associations between the different monitored substances as well as between levels determined in the different investigated biological matrices mostly do not appear statistically significant. The estimated materno-foetal transfer would be thus substance-dependant, mainly driven by the physico-chemical properties of the different PFAAs (nature of polar group and length of alkylated side chain). We conclude that trans-placental passage and breastfeeding are both significant routes of human exposure to PFAAs.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150728

TA - Environ Int

JT - Environment international

JID - 7807270

OTO - NOTNLM

OT - Biomonitoring

OT - Endocrine disruptors

OT - Perfluoroalkyl substances

OT - Perinatal exposure

OT - Profiling

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AID - 10.1016/j.envint.2015.07.014 [doi]

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SO - Environ Int. 2015 Jul 28;84:71-81. doi: 10.1016/j.envint.2015.07.014.

PMID- 26085281

OWN - NLM

STAT- In-Process

DA - 20150618

IS - 1573-2959 (Electronic)

IS - 0167-6369 (Linking)

VI - 187

IP - 7

DP - 2015 Jul

TI - Perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA): emerging

contaminants of increasing concern in fish from Lake Varese, Italy.

PG - 438

LID - 10.1007/s10661-015-4686-0 [doi]

AB - Perfluoroalkylated substances (PFASs) are highly fluorinated aliphatic compounds with high thermal and chemical stability, used in a range of industrial applications. Extensive screening analyses in biota samples from all over the world have shown the bioaccumulation of PFAS into higher trophic levels in the food chain. Perfluorooctane sulfonic acid (PFOS) and perfluorooctanoic acid (PFOA) are potential reproductive and developmental toxicants and are considered to be emerging endocrine disrupters. Ingestion of fish and other seafood is considered the main source of exposure of these contaminants. Here, we quantified PFOS and PFOA by LC-MS/MS in muscle samples of European perch from Lake Varese, Italy. PFOS was detected in all samples with concentrations of up to 17.2 ng g<sup>-1</sup>. Although the reported values were lower than the recommended total daily intake (TDI) proposed by the European Food Safety Authority (EFSA), fish from Lake Varese may be a significant source of dietary PFOS exposure.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150618

PL - Netherlands

TA - Environ Monit Assess

JT - Environmental monitoring and assessment

JID - 8508350

SB - IM

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PST - ppublish

SO - Environ Monit Assess. 2015 Jul;187(7):438. doi: 10.1007/s10661-015-4686-0. Epub 2015 Jun 18.

PMID- 26160670

OWN - NLM

STAT- Publisher

DA - 20150710

LR - 20150715

IS - 1873-6424 (Electronic)

IS - 0269-7491 (Linking)

VI - 206

DP - 2015 Jul 6

TI - Characterizing direct emissions of perfluoroalkyl substances from ongoing fluoropolymer production sources: A spatial trend study of Xiaoqing River, China.

PG - 104-112

LID - S0269-7491(15)00328-0 [pii]

LID - 10.1016/j.envpol.2015.06.035 [doi]

AB - The spatial trend of perfluoroalkyl substances (PFASs) along Xiaoqing River and its tributaries was studied to characterize isomer profiles and quantify emissions from fluoropolymer (FP) manufacturers in China. Substantially elevated summation operatorPFAS concentrations downstream of tributary 4 demonstrated that the emissions from this FP manufacturer dominated total riverine discharges. Isomer profiles of perfluorooctanoic acid (PFOA) in water displayed a stepwise increase in percentage branched PFOA downstream of tributary 3 (14.0%) and 4 (22.7%) reflecting the importance of FP sources. Strong positive correlations between PFOA isomers in water downstream of tributary 4 indicated that isomer profiles were conserved from emission sources to the final reservoir. Riverine discharges of PFOA (23-67 t/yr) were in agreement with theoretical emission calculations from FP production (68 t/yr) whereas large discrepancies between the two methodologies were observed for perfluorobutanoic acid and perfluoropentanoic acid. Collectively, this study fills critical knowledge gaps for understanding ongoing global sources of PFASs.

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 LA - ENG  
 PT - JOURNAL ARTICLE  
 DEP - 20150706  
 TA - Environ Pollut  
 JT - Environmental pollution (Barking, Essex : 1987)  
 JID - 8804476  
 OTO - NOTNLM  
 OT - Isomer fractionation  
 OT - PFOA isomers  
 OT - Per- and polyfluoroalkyl substances (PFASs)  
 OT - Source tracking  
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 SO - Environ Pollut. 2015 Jul 6;206:104-112. doi: 10.1016/j.envpol.2015.06.035.  
  
 PMID- 25827692  
 OWN - NLM  
 STAT- In-Process  
 DA - 20150429  
 IS - 1873-6424 (Electronic)  
 IS - 0269-7491 (Linking)  
 VI - 202

DP - 2015 Jul

TI - Adsorption of perfluoroalkyl acids by carbonaceous adsorbents: Effect of carbon surface chemistry.

PG - 168-76

LID - 10.1016/j.envpol.2015.03.019 [doi]

LID - S0269-7491(15)00141-4 [pii]

AB - Adsorption by carbonaceous sorbents is among the most feasible processes to remove perfluorooctane sulfonic (PFOS) and carboxylic acids (PFOA) from drinking and ground waters. However, carbon surface chemistry, which has long been recognized essential for dictating performance of such sorbents, has never been considered for PFOS and PFOA adsorption. Thus, the role of surface chemistry was systematically investigated using sorbents with a wide range in precursor material, pore structure, and surface chemistry. Sorbent surface chemistry overwhelmed physical properties in controlling the extent of uptake. The adsorption affinity was positively correlated carbon surface basicity, suggesting that high acid neutralizing or anion exchange capacity was critical for substantial uptake of PFOS and PFOA. Carbon polarity or hydrophobicity had insignificant impact on the extent of adsorption. Synthetic polymer-based Ambersorb and activated carbon fibers were more effective than activated carbon made of natural materials in removing PFOS and PFOA from aqueous solutions.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150330

PL - England

TA - Environ Pollut

JT - Environmental pollution (Barking, Essex : 1987)

JID - 8804476

SB - IM

OTO - NOTNLM

OT - Activated carbon fibers

OT - Basicity

OT - Carbonaceous sorbents

OT - PFOA

OT - PFOS

OT - Surface chemistry

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AID - 10.1016/j.envpol.2015.03.019 [doi]  
PST - ppublish  
SO - Environ Pollut. 2015 Jul;202:168-76. doi: 10.1016/j.envpol.2015.03.019. Epub 2015 Mar 30.

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OWN - NLM

STAT- In-Process

DA - 20150429

IS - 1873-6424 (Electronic)

IS - 0269-7491 (Linking)

VI - 202

DP - 2015 Jul

TI - Estimating dry deposition and gas/particle partition coefficients of neutral poly-/perfluoroalkyl substances in northern German coast.

PG - 120-5

LID - 10.1016/j.envpol.2015.03.029 [doi]

LID - S0269-7491(15)00159-1 [pii]

AB - Dry deposition fluxes of 12 neutral poly-/perfluoroalkyl substances (PFASs) were estimated at Busum located in northern German coast, and their gas/particle partition coefficients were predicted by employing the polyparameter linear free energy relationships (PP-LFERs). The gas deposition flux, particle deposition flux and total (gas + particle) flux of the 12 PFASs during sampling periods were 1088 +/- 611, 189 +/- 75 and 1277 +/- 627 pg/(m(2) d), respectively. The gas deposition of PFASs played a key role during deposition to marine ecosystem. Sensitivity analysis showed that wind speed was the most sensitive parameter for gas deposition fluxes. Good agreements (within 1 log unit) were observed between the measured gas/particle partitioning data of PFASs and the predicted partition coefficients using PP-LFERs, indicating the model can reliably predict the gas/particle partitioning behaviors of atmospheric neutral PFASs.

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LA - eng  
PT - Journal Article  
PT - Research Support, Non-U.S. Gov't  
DEP - 20150326  
PL - England  
TA - Environ Pollut  
JT - Environmental pollution (Barking, Essex : 1987)  
JID - 8804476  
SB - IM  
OTO - NOTNLM  
OT - 8:2 FTOH  
OT - Gas diffusive deposition  
OT - Gas/particle partition coefficients  
OT - PFASs  
OT - PP-LFERS  
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AID - S0269-7491(15)00159-1 [pii]  
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SO - Environ Pollut. 2015 Jul;202:120-5. doi: 10.1016/j.envpol.2015.03.029. Epub 2015 Mar 26.  
  
PMID- 26142720  
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DA - 20150705  
LR - 20150706  
IS - 1096-0953 (Electronic)  
IS - 0013-9351 (Linking)  
VI - 142

DP - 2015 Jul 2

TI - Levels of perfluoroalkyl substances and risk of coronary heart disease: Findings from a population-based longitudinal study.

PG - 148-154

LID - S0013-9351(15)30013-X [pii]

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AB - BACKGROUND: Cross-sectional studies have shown an association between exposure to perfluoroalkyl substances (PFASs) and coronary heart disease (CHD). These findings need to be evaluated in longitudinal settings. OBJECTIVES: To investigate the risk of CHD in relation to PFAS levels in a longitudinal setting among Swedish rural residents. METHODS: In a population-based prospective cohort of male farmers and rural residents recruited in 1990-1991, all men who received a CHD diagnosis between 1992 and 2009 were identified from national registers (n=253). For each CHD case, one control, matched for age, was chosen randomly from the cohort. For all cases and controls, levels of eight PFASs at baseline were measured in stored blood samples. In addition, for a subsample, PFAS levels were also measured in serum samples collected at a follow-up in 2002-2003. RESULTS: There were no statistically significant associations between levels of seven of the eight PFASs at baseline and risk for developing CHD. There was a significant association between perfluoroheptanoic acid (PFHpA) and CHD (OR=2.72; 95% CI: 1.52, 4.84) for the 3rd quartile and (OR=2.45; 95% CI: 1.40, 4.29) for the 4th quartile compared to the lowest quartile. Changes in levels of PFCs between baseline and follow-up did not differ systematically between cases and controls. CONCLUSIONS: This longitudinal study does not lend support to the previously reported cross-sectional relationship between PFAS levels and CHD risk. We found a significant association with PFHpA, but this could be a chance finding, considering its chemical resemblance to other PFASs.

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 TI - Influence of contaminated drinking water on perfluoroalkyl acid levels in human  
 serum - A case study from Uppsala, Sweden.  
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 AB - In 2012 a contamination of drinking water with perfluoroalkyl acids (PFAAs) was

uncovered in the City of Uppsala, Sweden. The aim of the present study was to determine how these substances have been distributed from the contamination source through the groundwater to the drinking water and how the drinking water exposure has influenced the levels of PFAAs in humans over time. The results show that PFAA levels in groundwater measured 2012–2014 decreased downstream from the point source, although high SigmaPFAA levels (>100ng/L) were still found several kilometers from the point source in the Uppsala aquifer. The usage of aqueous film forming fire-fighting foams (AFFF) at a military airport in the north of the city is probably an important contamination source. Computer simulation of the distribution of PFAA-contaminated drinking water throughout the City using a hydraulic model of the pipeline network suggested that consumers in the western and southern parts of Uppsala have received most of the contaminated drinking water. PFAA levels in blood serum from 297 young women from Uppsala County, Sweden, sampled during 1996–1999 and 2008–2011 were analyzed. Significantly higher concentrations of perfluorobutane sulfonic acid (PFBS) and perfluorohexane sulfonic acid (PFHxS) were found among women who lived in districts modeled to have received contaminated drinking water compared to unaffected districts both in 1996–1999 and 2008–2011, indicating that the contamination was already present in the late 1990s. Isomer-specific analysis of PFHxS in serum showed that women in districts with contaminated drinking water also had an increased percentage of branched isomers. Our results further indicate that exposure via contaminated drinking water was the driving factor behind the earlier reported increasing temporal trends of PFBS and PFHxS in blood serum from young women in Uppsala.

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AB - The potential toxicity of background exposure to perfluoroalkyl substances (PFASs) is currently under active investigation. Such investigations typically rely on a single measure of PFAS concentration, yet the longer-term reliability of a single measure has not been well characterized, especially among reproductive-aged women. Our aim was to investigate the association between PFAS plasma concentrations of 100 women in two consecutive pregnancies and explore changes in plasma concentration related to reproductive factors. The women in our study were enrolled in the Norwegian Mother and Child Cohort Study (MoBa) from 2003 to 2009. About half of them breastfed exclusively for 6 months and the rest of the participants did not breastfeed between the two consecutive pregnancies (median time between pregnancies: 18 months). Maternal blood was collected at mid-pregnancy and plasma was analyzed for 10 PFASs. Statistical analyses were restricted to 6 PFASs that were quantifiable in more than 80% of the samples. We estimated the correlation between repeated PFAS measurements, the percentage change between pregnancies and the effect of several reproductive factors in multivariate linear regression models of PFAS concentrations in the second pregnancy. The Pearson correlation coefficient between repeated PFAS measurements was, for perfluorooctane sulfonate (PFOS), 0.80; perfluorooctanoate (PFOA), 0.50; perfluorohexane sulfonate (PFHxS), 0.74; perfluorononanoate (PFNA), 0.39; perfluoroundecanoate (PFUnDA), 0.71; and perfluorodecanoate (PFDA), 0.60. Adjustment for maternal age, delivery year, and time and breastfeeding between pregnancies did not substantially affect the observed correlations. We found 44-47% median reductions in the concentrations of PFOS, PFOA and PFHxS between pregnancies, while the change in concentrations between pregnancies was smaller and more variable for PFNA, PFUnDA and PFDA. The variation in plasma concentrations in the second pregnancy was mainly accounted for by the concentration in the first pregnancy; for PFOS, PFOA, and PFNA, breastfeeding also accounted for a substantial proportion. In conclusion, we found the reliability of PFAS measurements in maternal plasma to be moderate to high, and in these data, several factors, especially breastfeeding, were related to plasma concentrations.

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 TI - Prenatal exposure to phthalates, bisphenol A and perfluoroalkyl substances and

cord blood levels of IgE, TSLP and IL-33.

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AB - The fetal time period is a critical window of immune system development and resulting heightened susceptibility to the adverse effects of environmental exposures. Epidemiologists and toxicologists have hypothesized that phthalates, bisphenol A (BPA) and perfluoroalkyl substance have immunotoxic properties. Immunotoxic effects of chemicals may manifest in an altered immune system profile at birth. Immunoglobulin E, thymic stromal lymphopoietin (TSLP), and interleukin-33 (IL-33) are integral in the etiology of childhood allergy and detectable at birth. The objective of this study was to determine the association between maternal levels of phthalates, bisphenol A (BPA), and perfluoroalkyl substances and elevated umbilical cord blood levels of IgE, TSLP, and IL-33. This study utilized data collected in the Maternal-Infant Research on Environmental Chemicals (MIREC) Study, a trans-Canada cohort study of 2001 pregnant women. Of these women, 1258 had a singleton, term birth and cord blood sample. A Bayesian hierarchical model was employed to determine associations between log-transformed continuous variables and immune system biomarkers while adjusting for potential confounding from correlated environmental contaminants. Inverse, nonlinear associations were observed between maternal urinary MCPP levels and elevated levels of both IL-33/TSLP and IgE and between maternal urinary BPA levels and elevated levels of IL-33/TSLP. In this primarily urban Canadian population of pregnant women and their newborns, maternal urinary and plasma concentrations of phthalate metabolites, BPA, and perfluoroalkyl substances were not associated with immunotoxic effects that manifest as increased odds of elevated levels of IgE, TSLP or IL-33.

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 TI - Physiologically-based pharmacokinetic modelling of immune, reproductive and  
 carcinogenic effects from contaminant exposure in polar bears (Ursus maritimus)

across the Arctic.

PG - 45-55

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AB - Polar bears (*Ursus maritimus*) consume large quantities of seal blubber and other high trophic marine mammals and consequently have some of the highest tissue concentrations of organohalogen contaminants (OHCs) among Arctic biota. In the present paper we carried out a risk quotient (RQ) evaluation on OHC-exposed polar bears harvested from 1999 to 2008 and from 11 circumpolar subpopulations spanning from Alaska to Svalbard in order to evaluate the risk of OHC-mediated reproductive effects (embryotoxicity, teratogenicity), immunotoxicity and carcinogenicity (genotoxicity). This RQ evaluation was based on the Critical Body Residue (CBR) concept and a Physiologically-Based Pharmacokinetic Modelling (PBPK) approach using OHC concentrations measured in polar bear adipose or liver tissue. The range of OHC concentrations within polar bear populations were as follows for adipose, sum polychlorinated biphenyls summation operatorPCBs (1797-10,537ng/g lw), sum methylsulphone-PCB summation operatorMeSO<sub>2</sub>-PCBs (110-672ng/g lw), sum chlordanes summation operatorCHLs (765-3477ng/g lw), alpha-hexachlorocyclohexane alpha-HCH (8.5-91.3ng/g lw), beta-hexachlorocyclohexane beta-HCH (65.5-542ng/g lw), sum chlorbenzenes summation operatorClBzs (145-304ng/g lw), dichlorodiphenyltrichloroethane summation operatorDDTs (31.5-206ng/g lw), dieldrin (69-249ng/g lw), polybrominated diphenyl ethers summation operatorPBDEs (4.6-78.4ng/g lw). For liver, the perfluorooctanesulfonic acid (PFOS) concentrations ranged from 231-2792ng/g ww. The total additive RQ from all OHCs ranged from 4.3 in Alaska to 28.6 in East Greenland bears for effects on reproduction, immune health and carcinogenicity, highlighting the important result that the toxic effect threshold (i.e. RQ>1) was exceeded for all polar bear populations assessed. PCBs were the main contributors for all three effect categories, contributing from 70.6% to 94.3% of the total risk and a RQ between 3.8-22.5. summation operatorMeSO<sub>2</sub>-PCBs were the second highest effect contributor for reproductive and immunological effects (0.17<RQ<1.4), whereas PFOS was the second highest effect contributor for carcinogenic (genotoxic) effects (0.35<RQ<2.5). The results from this study corroborate and lend further support to previous assessments of the possible adverse health effects of exposure to known and measured OHCs in polar bears. We therefore suggest that Critical Daily Doses (CDD) should be investigated in "ex vivo" dose-response studies on polar bears to replace laboratory studies on rats (*Rattus rattus*) to reveal whether high RQs are maintained.

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TI - Urinary heavy metals, phthalates and polyaromatic hydrocarbons independent of health events are associated with adult depression: USA NHANES, 2011-2012.

AB - Links between environmental chemicals and human health have emerged, but the effects on mental health such as depression were less studied. Therefore, it was aimed to study the relationships between different sets of urinary environmental chemical concentrations and adult depression in a national and population-based setting in recent years. Data was retrieved from the US National Health and Nutrition Examination Survey in 2011-2012 including demographics, serum measurements, lifestyle factors, self-reported health conditions and urinary chemical concentrations. Depression was determined by using the Patient Health Questionnaire with a cutoff point at 9/10. Chi-square test, t test and survey-weighted logistic regression modeling were performed. Among 5560 American adults aged 20-80 years, 363 (7.8 %) people were classified as having depression (Patient Health Questionnaire score  $\geq 10$ ). They tended to have history of health events. After full adjustment including urinary creatinine; demographic characteristics; lifestyle factors; health conditions (such as cardiovascular, neurological, respiratory, digestive and bone diseases, and injury); and subsample weighing; and higher levels of manganese, tin, and phthalates including mono-2-ethyl-5-carboxypentyl, mono-n-butyl, mono-isobutyl, and mono-benzyl were associated with adult depression. Similarly, urinary polyaromatic hydrocarbons including 2-hydroxyfluorene, 3-hydroxyfluorene, 9-hydroxyfluorene, 1-hydroxyphenanthrene, 2-hydroxyphenanthrene, 3-hydroxyphenanthrene, 1-hydroxypyrene, 1-hydroxynaphthalene (1-naphthol), 2-hydroxynaphthalene (2-naphthol) and 4-hydroxyphenanthrene were associated with depression. There were no associations observed in urinary arsenic, phenols, parabens, pesticides, perchlorate, nitrate, thiocyanate and polyfluorinated compounds. Urinary heavy metal, phthalates and polyaromatic hydrocarbons were associated with adult

depression, being independent of health events. Further elimination of such harmful chemicals might need to be considered in future mental health and environmental policies.

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TI - Perfluoroalkyl substances in the Daling River with concentrated fluorine industries in China: seasonal variation, mass flow, and risk assessment.

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LID - 10.1007/s11356-015-4189-0 [doi]

AB - In the present study, we investigated concentrations and composition profiles of perfluoroalkyl substances (PFASs) in surface water from the Daling River in different seasons. The highest concentration of SigmaPFASs (9540 ng L<sup>-1</sup>) and dominant homologues were found in surface water collected in summer. Perfluorobutanoic acid (PFBA), perfluorobutane sulfonate (PFBS), and perfluorooctanoic acid (PFOA) were the dominant PFASs in four seasons with a total contribution of over 90 %. The discharge of two fluorine chemical industry parks was predicted to be the main contamination source of PFASs in the study area. The daily and annual mass flows were calculated according to data of detected PFAS concentrations and water discharge, and the annual mass loading of PFASs into the Bohai Sea from the Daling River reached to 461 kg year<sup>-1</sup>. Hazard assessment indicated that concentrations of PFASs in study area had little risk

to aquatic organisms and wildlife. However, the multiple health risk would be relatively high if the water was served as drinking water in the study area.

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AU - Wang P

FAU - Li, Qifeng

AU - Li Q

FAU - Lu, Yonglong

AU - Lu Y

LA - eng

PT - Journal Article

DEP - 20150211

PL - Germany

TA - Environ Sci Pollut Res Int

JT - Environmental science and pollution research international

JID - 9441769

SB - IM

EDAT- 2015/02/11 06:00

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PHST- 2015/02/11 [aheadofprint]

AID - 10.1007/s11356-015-4189-0 [doi]

PST - ppublish

SO - Environ Sci Pollut Res Int. 2015 Jul;22(13):10009-18. doi:  
10.1007/s11356-015-4189-0. Epub 2015 Feb 11.

PMID- 25616381

OWN - NLM

STAT- In-Data-Review

DA - 20150627

IS - 1614-7499 (Electronic)

IS - 0944-1344 (Linking)

VI - 22

IP - 13

DP - 2015 Jul

TI - Transport of short-chain perfluoroalkyl acids from concentrated fluoropolymer  
facilities to the Daling River estuary, China.

PG - 9626-36

LID - 10.1007/s11356-015-4090-x [doi]

AB - After global commercialization of short-chain perfluoroalkyl acids (PFAAs) as substitutes to conventional long-chain PFAAs by the major manufacturers, two fluorine industry parks for production of short-chain PFAAs located in the Daling River Basin of northern China have developed rapidly in the last few years. This study provides a systematic assessment of sources, emissions, transportation, and potential risks of the PFAAs in this area. The C4 perfluorobutane sulfonic acid (PFBS) and perfluorobutanoic acid (PFBA) were the predominant short-chain PFAAs in river water, with maximum concentrations of 2.90 and 1.35 µg/L, respectively. Park 1 equipped with a telomerization process was identified to be the source of linear and branched mixtures of PFBS, PFBA, and perfluorooctanoic acid (PFOA), while park 2 with an electrochemical fluorination process (ECF) was identified to be the source of linear and branched mixtures of PFBS and PFOA. Partition coefficients between water and sediment were consistent for C4-C8 perfluoroalkyl carboxylic acids (PFCAs) but directly proportional to C9-C11 PFCAs and perfluoroalkyl sulfonic acids (PFSA). Analysis on the health risk of PFBS and PFBA suggested that they were not without risk since short chain PFAAs are known to be recalcitrant during water treatment.

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FAU - Giesy, John P

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LA - eng

PT - Journal Article

DEP - 20150124

PL - Germany

TA - Environ Sci Pollut Res Int

JT - Environmental science and pollution research international

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SB - IM

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 PHST- 2015/01/07 [accepted]  
 PHST- 2015/01/24 [aheadofprint]  
 AID - 10.1007/s11356-015-4090-x [doi]  
 PST - ppublish  
 SO - Environ Sci Pollut Res Int. 2015 Jul;22(13):9626-36. doi:  
 10.1007/s11356-015-4090-x. Epub 2015 Jan 24.

PMID- 26055930  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150707  
 IS - 1520-5851 (Electronic)  
 IS - 0013-936X (Linking)  
 VI - 49  
 IP - 13  
 DP - 2015 Jul 7  
 TI - Physical and Biological Release of Poly- and Perfluoroalkyl Substances (PFASs)  
 from Municipal Solid Waste in Anaerobic Model Landfill Reactors.  
 PG - 7648-56  
 LID - 10.1021/acs.est.5b01040 [doi]  
 AB - A wide variety of consumer products that are treated with poly- and  
 perfluoroalkyl substances (PFASs) and related formulations are disposed of in  
 landfills. Landfill leachate has significant concentrations of PFASs and acts as  
 secondary point sources to surface water. This study models how PFASs enter  
 leachate using four laboratory-scale anaerobic bioreactors filled with municipal  
 solid waste (MSW) and operated over 273 days. Duplicate reactors were monitored  
 under live and abiotic conditions to evaluate influences attributable to  
 biological activity. The biologically active reactors simulated the methanogenic  
 conditions that develop in all landfills, producing approximately 140 mL CH<sub>4</sub>/dry  
 g refuse. The average total PFAS leaching measured in live reactors (16.7 nmol/kg  
 dry refuse) was greater than the average for abiotic reactors (2.83 nmol/kg dry  
 refuse), indicating biological processes were primarily responsible for leaching.  
 The low-level leaching in the abiotic reactors was primarily due to PFCAs  $\leq$  C<sub>8</sub>  
 (2.48 nmol/kg dry refuse). Concentrations of known biodegradation intermediates,  
 including methylperfluorobutane sulfonamide acetic acid and the n:2 and n:3  
 fluorotelomer carboxylates, increased steadily after the onset of methanogenesis,  
 with the 5:3 fluorotelomer carboxylate becoming the single most concentrated PFAS  
 observed in live reactors (9.53 nmol/kg dry refuse).

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PT - Journal Article  
DEP - 20150625  
PL - United States  
TA - Environ Sci Technol  
JT - Environmental science & technology  
JID - 0213155  
SB - IM  
EDAT- 2015/06/10 06:00  
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PHST- 2015/06/25 [aheadofprint]  
AID - 10.1021/acs.est.5b01040 [doi]  
PST - ppublish  
SO - Environ Sci Technol. 2015 Jul 7;49(13):7648-56. doi: 10.1021/acs.est.5b01040.  
Epub 2015 Jun 25.  
  
PMID- 26042823  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150707  
IS - 1520-5851 (Electronic)  
IS - 0013-936X (Linking)  
VI - 49  
IP - 13  
DP - 2015 Jul 7  
TI - Aerobic Biotransformation of Fluorotelomer Thioether Amido Sulfonate (Lodyne) in  
AFFF-Amended Microcosms.  
PG - 7666-74  
LID - 10.1021/acs.est.5b01219 [doi]  
AB - The aerobic biotransformation pathways of 4:2, 6:2, and 8:2 fluorotelomer  
thioether amido sulfonate (FtTAoS) were characterized by determining the fate of  
the compounds in soil and medium microcosms amended with an aqueous film-forming  
foam (AFFF) solution. The biotransformation of FtTAoS occurred in live microcosms  
over approximately 40 days and produced 4:2, 6:2, and 8:2 fluorotelomer sulfonate  
(FtS), 6:2 fluorotelomer unsaturated carboxylic acid (FtUCA), 5:3 fluorotelomer  
carboxylic acid (FtCA), and C4 to C8 perfluorinated carboxylic acids (PFCAs). Two  
biotransformation products corresponding to singly and doubly oxygenated forms of

6:2 FtTAoS were also identified through high resolution mass spectrometry (MS) analysis and liquid chromatography tandem-MS. An oxidative assay was used to indirectly quantify the total concentration of polyfluorinated compounds and check the mass balance. The assay produced near complete mass recovery of FtTAoS after biotransformation, with 10% (mol/mol) of the amended FtTAoS accounted for in FtS, FtCA, and PFCA products. The transformation rates of identified products appear to be slow relative to FtTAoS, indicating that some intermediates may persist in the environment. This study confirms some of the sources of FtS and PFCAs in groundwater and soil at AFFF-impacted sites and suggests that fluorinated intermediates that are not routinely measured during the biotransformation of PFASs may accumulate.

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LA - eng

PT - Journal Article

DEP - 20150623

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

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EDAT- 2015/06/05 06:00

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PHST- 2015/06/23 [aheadofprint]  
 AID - 10.1021/acs.est.5b01219 [doi]  
 PST - ppublish  
 SO - Environ Sci Technol. 2015 Jul 7;49(13):7666-74. doi: 10.1021/acs.est.5b01219.  
 Epub 2015 Jun 23.

PMID- 26106903  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150721  
 IS - 1520-5851 (Electronic)  
 IS - 0013-936X (Linking)  
 VI - 49  
 IP - 14  
 DP - 2015 Jul 21  
 TI - Alternative and Legacy Perfluoroalkyl Substances: Differences between European  
 and Chinese River/Estuary Systems.  
 PG - 8386-95  
 LID - 10.1021/acs.est.5b01648 [doi]  
 AB - The production and use of long-chain perfluoroalkyl substances (PFASs) must  
 comply with national and international regulations. Driven by increasingly  
 stringent regulations, their production has been outsourced to less regulated  
 countries in Asia. In addition, the fluoropolymer industry started to use  
 fluorinated alternatives, such as  
 2,3,3,3-tetrafluoro-2-(1,1,2,2,3,3,3-heptafluoropropoxy)propanoic acid (HFPO-DA).  
 Between August 2013 and September 2014, we investigated the occurrence and  
 distribution of HFPO-DA and legacy PFASs in surface waters of the following  
 river/estuary systems: the Elbe and Rhine Rivers in Germany, the Rhine-Meuse  
 delta in The Netherlands, and the Xiaoqing River in China. Distinct differences  
 were revealed among the study areas; notably, the Chinese samples were highly  
 polluted by an industrial point source discharging mainly perfluorooctanoic acid  
 (PFOA). This particular point source resulted in concentrations more than 6000  
 times higher than an industrial point source observed in the Schuur River, where  
 HFPO-DA was the dominant compound with a concentration of 73.1 ng/L. Moreover,  
 HFPO-DA was detected in all samples along the coastline of the North Sea,  
 indicating that the compound may be transported from the Rhine-Meuse delta into  
 the German Bight via the water current. To the best of our knowledge, the  
 fluorinated alternative, HFPO-DA, was detected for the first time in surface  
 waters of Germany and China.

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LA - eng

PT - Journal Article

DEP - 20150707

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM

EDAT- 2015/06/25 06:00

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PHST- 2015/07/07 [aheadofprint]

AID - 10.1021/acs.est.5b01648 [doi]

PST - ppublish

SO - Environ Sci Technol. 2015 Jul 21;49(14):8386-95. doi: 10.1021/acs.est.5b01648. Epub 2015 Jul 7.

PMID- 26066631

OWN - NLM

STAT- In-Data-Review

DA - 20150721

IS - 1520-5851 (Electronic)

IS - 0013-936X (Linking)

VI - 49

IP - 14

DP - 2015 Jul 21

TI - Understanding the Adsorption of PFOA on MIL-101(Cr)-Based Anionic-Exchange Metal-Organic Frameworks: Comparing DFT Calculations with Aqueous Sorption Experiments.

PG - 8657-65

LID - 10.1021/acs.est.5b00802 [doi]

AB - To examine the effects of different functionalization methods on adsorption behavior, anionic-exchange MIL-101(Cr) metal-organic frameworks (MOFs) were synthesized using preassembled modification (PAM) and postsynthetic modification (PSM) methods. Perfluorooctanoic acid (PFOA) adsorption results indicated that

the maximum PFOA adsorption capacity was 1.19 and 1.89 mmol g<sup>(-1)</sup> for anionic-exchange MIL-101(Cr) prepared by PAM and PSM, respectively. The sorption equilibrium was rapidly reached within 60 min. Our results indicated that PSM is a better modification technique for introducing functional groups onto MOFs for adsorptive removal because PAM places functional groups onto the aperture of the nanopore, which hinders the entrance of organic contaminants. Our experimental results and the results of complementary density functional theory calculations revealed that in addition to the anion-exchange mechanism, the major PFOA adsorption mechanism is a combination of Lewis acid/base complexation between PFOA and Cr(III) and electrostatic interaction between PFOA and the protonated carboxyl groups of the bdc (terephthalic acid) linker.

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LA - eng

PT - Journal Article

DEP - 20150702

PL - United States

TA - Environ Sci Technol

JT - Environmental science & technology

JID - 0213155

SB - IM  
 EDAT- 2015/06/13 06:00  
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 CRDT- 2015/06/13 06:00  
 PHST- 2015/07/02 [aheadofprint]  
 AID - 10.1021/acs.est.5b00802 [doi]  
 PST - ppublish  
 SO - Environ Sci Technol. 2015 Jul 21;49(14):8657-65. doi: 10.1021/acs.est.5b00802.  
 Epub 2015 Jul 2.

PMID- 25772371  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150629  
 IS - 1552-8618 (Electronic)  
 IS - 0730-7268 (Linking)  
 VI - 34  
 IP - 7  
 DP - 2015 Jul  
 TI - Uptake of perfluoroalkyl acids in the leaves of coniferous and deciduous  
 broad-leaved trees.  
 PG - 1499-504  
 LID - 10.1002/etc.2968 [doi]  
 AB - Analytical methods for determining perfluoroalkyl acids (PFAAs) in leaves were  
 developed to quantify a suite of analytes in both coniferous and deciduous  
 broad-leaved trees. Sodium hydroxide-methanol and solid-phase extraction was  
 selected as the extracting and cleanup strategy for PFAA analysis. Ten  
 perfluorocarboxylic acids (PFCAs) and 4 perfluorosulfonic acids (PFSAs) were  
 monitored in 7 kinds of leaves grown in the urban areas of Dalian, China. The  
 results show that coniferous tree leaves take up more PFAAs than broad-leaved  
 tree leaves, with the highest amount of 150 ng/g in pine needles. Leaf PFCA  
 levels were much higher than PFSAs level. Short carbon-chain PFCAs with 3 to 6  
 perfluorinated carbons account for approximately 40% to 80% of the total leaf  
 PFAAs, where uptake decreased with increasing carbon chain length. Temporal  
 observation of leaf PFAAs revealed no significant variation of concentrations in  
 the leaves over a weekly interval and the absence of significant seasonal change  
 in pine needles and sophora. The present study provides some evidence for the  
 accumulation of PFAAs in leaves, which is valuable for understanding their  
 environmental behavior and the development of alternative bioindicator. Environ  
 Toxicol Chem 2015;34:1499-1504. (c) 2015 SETAC.  
 CI - (c) 2015 SETAC.  
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LA - eng

PT - Journal Article

DEP - 20150505

PL - United States

TA - Environ Toxicol Chem

JT - Environmental toxicology and chemistry / SETAC

JID - 8308958

SB - IM

OTO - NOTNLM

OT - Bioaccumulation

OT - Biomonitoring

OT - Environmental transport

OT - Perfluoroalkyl substance

OT - Plant

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AID - 10.1002/etc.2968 [doi]

PST - ppublish

SO - Environ Toxicol Chem. 2015 Jul;34(7):1499-504. doi: 10.1002/etc.2968. Epub 2015 May 5.

PMID- 25677940

OWN - NLM

STAT- In-Data-Review

DA - 20150629

IS - 1552-8618 (Electronic)

IS - 0730-7268 (Linking)

VI - 34

IP - 7

DP - 2015 Jul

TI - Circumpolar contamination in eggs of the high-arctic ivory gull *Pagophila eburnea*.

PG - 1552-61

LID - 10.1002/etc.2935 [doi]

AB - The ivory gull *Pagophila eburnea* is a high-Arctic species threatened by climate change and contaminants. The objective of the present study was to assess spatial variation of contaminant levels (organochlorines [OCs], brominated flame retardants [BFRs], perfluorinated alkyl substances [PFASs], and mercury [Hg]) in ivory gulls breeding in different areas across the Arctic region as a baseline for potential future changes associated with climate change. Contaminants were already determined in eggs from Canada (Seymour Island; except PFASs), Svalbard in Norway (Svenskoya), and 3 sites in Russia (Nagurskoe, Cape Klyuv, and Domashny). New data from Greenland allowed the investigation of a possible longitudinal gradient of contamination. The most quantitatively abundant OCs were p,p'-dichlorodiphenyldichloroethylene (DDE) and polychlorobiphenyls. Mercury concentrations were higher in Canada compared with other colonies. Eggs from Nagurskoe often were characterized by higher OC and BFR concentrations. Concentrations gradually decreased in colonies situated east of Nagurskoe. In contrast, PFAS concentrations, especially perfluorooctanoate and perfluorononanoate, were higher in Greenland. Some of the contaminants, especially Hg and p,p'-DDE, exceeded published thresholds known to disrupt the reproductive success of avian species. Overall, the levels of OCs, BFRs, and PFASs did not suggest direct lethal exposure to these compounds, but their potential synergetic/additive sublethal effects warrant monitoring. *Environ Toxicol Chem* 2015;34:1552-1561. (c) 2015 SETAC.

CI - (c) 2015 SETAC.

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 LA - eng  
 PT - Journal Article  
 DEP - 20150505  
 PL - United States  
 TA - Environ Toxicol Chem  
 JT - Environmental toxicology and chemistry / SETAC  
 JID - 8308958  
 SB - IM  
 OTO - NOTNLM  
 OT - Arctic  
 OT - Ivory gull  
 OT - Perfluorinated alkyl substances  
 OT - Persistent organic pollutants  
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 AID - 10.1002/etc.2935 [doi]  
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 SO - Environ Toxicol Chem. 2015 Jul;34(7):1552-61. doi: 10.1002/etc.2935. Epub 2015  
 May 5.  
  
 PMID- 26254212  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150808  
 LR - 20150809  
 IS - 1872-7077 (Electronic)  
 IS - 1382-6689 (Linking)  
 VI - 40  
 IP - 2  
 DP - 2015 Jul 18  
 TI - More signs of neurotoxicity of surfactants and flame retardants - Neonatal PFOS  
 and PBDE 99 cause transcriptional alterations in cholinergic genes in the mouse

CNS.

PG - 409-416

LID - S1382-6689(15)30014-4 [pii]

LID - 10.1016/j.etap.2015.06.014 [doi]

AB - Maternally and lactationally transferred persistent organic pollutants may interfere with CNS development. Here, 10-day-old male mice were exposed to single oral doses of PFOS (perflourooctanosulphonate) or PBDE 99 (2,2',4,4',5-penta-bromodiphenyl ether), and examined for changes in cholinergic gene transcription in the CNS 24h and 7 weeks later. 24h after exposure qPCR analyses revealed decreased transcription of nAChR-beta2 and AChE in cortex, and increased mAChR-5 in hippocampus of PFOS treated mice. Neonatal PFOS treatment altered spontaneous behaviour at 2 months of age but did not affect gene transcription in adults. At 2 months of age neonatally PBDE 99 treated mice had altered spontaneous behaviour, and cortical transcription of AChE, nAChR-alpha4, nAChR-beta2 and mAChR-5 were elevated. Our results indicate that PFOS and PBDE 99 affects the developing central cholinergic system by altering gene transcription in cortex and hippocampus, which may in part account for mechanisms causing changes in spontaneous behaviour.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150718

TA - Environ Toxicol Pharmacol

JT - Environmental toxicology and pharmacology

JID - 9612020

OTO - NOTNLM

OT - Brain growth spurt

OT - Brominated flame retardants

OT - Cholinergic system

OT - Developmental neurotoxicology

OT - Perflourinated chemical repellants

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AID - S1382-6689(15)30014-4 [pii]  
AID - 10.1016/j.etap.2015.06.014 [doi]  
PST - aheadofprint  
SO - Environ Toxicol Pharmacol. 2015 Jul 18;40(2):409-416. doi:  
10.1016/j.etap.2015.06.014.

PMID- 25869105  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150627  
IS - 1633-8065 (Print)  
IS - 1633-8065 (Linking)  
VI - 25  
IP - 5  
DP - 2015 Jul  
TI - Nailing or plating for subtrochanteric femoral fractures: a non-randomized comparative study.  
PG - 889-94  
LID - 10.1007/s00590-015-1629-y [doi]  
AB - BACKGROUND: The aim of the present study was to compare the outcomes of reverse less invasive stabilization system for distal femur (LISS-DF) plates and proximal femoral nail antirotation (PFNA) in the treatment of patients with subtrochanteric fracture. METHODS: Thirty-one patients with 32 fractures were included in this study. The PFNA group consisted of 16 patients, and the reverse LISS-DF plate group consisted of 15 patients. Intraoperative data such as surgical time (min), amount of blood transfusion (units and erythrocyte suspensions) and radiation time (seconds) were noted. Time elapsed until fracture consolidation (weeks), time until full weight bearing (weeks), mean Harris hip score and length of stay (LOS) at hospital (days) were recorded postoperatively. RESULTS: The reverse LISS-DF group had a significantly longer elapsed time until fracture consolidation ( $p < 0.05$ ). The mean radiation time was significantly longer ( $p < 0.05$ ), and the Harris hip scores at last control were significantly higher ( $p < 0.05$ ) compared with the PFNA group. No significant differences were determined in terms of complications and re-operation rates. CONCLUSION: This study demonstrated that in the reverse LISS-DF-treated group, the mean time for bone union was longer and weight bearing was delayed. Considering the surgical technique, minimal surgical approach, reduced amount of blood transfusion and superior functional results following surgery, we concluded that the PFNA system offers advantages over reverse LISS-DF plating in the treatment of subtrochanteric femur fractures.

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FAU - Karapinar, Levent  
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 LA - eng  
 PT - Journal Article  
 DEP - 20150414  
 PL - France  
 TA - Eur J Orthop Surg Traumatol  
 JT - European journal of orthopaedic surgery & traumatology : orthopedie traumatologie  
 JID - 9518037  
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 AID - 10.1007/s00590-015-1629-y [doi]  
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 SO - Eur J Orthop Surg Traumatol. 2015 Jul;25(5):889-94. doi:  
 10.1007/s00590-015-1629-y. Epub 2015 Apr 14.  
  
 PMID- 26149266  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150806  
 IS - 1574-6968 (Electronic)  
 IS - 0378-1097 (Linking)  
 VI - 362  
 IP - 14  
 DP - 2015 Jul  
 TI - Cyclodepsipeptides produced by actinomycetes inhibit cyclic-peptide-mediated  
 quorum sensing in Gram-positive bacteria.  
 LID - 10.1093/femsle/fnv109 [doi]  
 LID - fnv109 [pii]  
 AB - Cyclic peptides are commonly used as quorum-sensing autoinducers in Gram-positive  
 Firmicutes bacteria. Well-studied examples of such molecules are thiolactone and  
 lactone, used to regulate the expression of a series of virulence genes in the  
 agr system of Staphylococcus aureus and the fsr system of Enterococcus faecalis,  
 respectively. Three cyclodepsipeptides WS9326A, WS9326B and cochinmicin II/III  
 were identified as a result of screening actinomycetes culture extracts for  
 activity against the agr/fsr system. These molecules are already known as  
 receptor antagonists, the first two for tachykinin and the last one for  
 endothelin. WS9326A also inhibited the transcription of pfoA regulated by the  
 VirSR two-component system in Clostridium perfringens. Receptor-binding assays  
 using a fluorescence-labeled autoinducer (FITC-GBAP) showed that WS9326A and  
 WS9326B act as receptor antagonists in this system. In addition, an ex vivo assay

showed that WS9326B substantially attenuated the toxicity of *S. aureus* for human corneal epithelial cells. These results suggest that these three natural cyclodepsipeptides have therapeutic potential for targeting the cyclic peptide-mediated quorum sensing of Gram-positive pathogens.

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LA - eng

PT - Journal Article

DEP - 20150705

PL - England

TA - FEMS Microbiol Lett

JT - FEMS microbiology letters

JID - 7705721

SB - IM

OTO - NOTNLM

OT - Enterococcus faecalis

OT - Staphylococcus aureus

OT - agr system

OT - cyclodepsipeptide

OT - fsr system

OT - quorum sensing inhibitor

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SO - FEMS Microbiol Lett. 2015 Jul;362(14). pii: fnv109. doi: 10.1093/femsle/fnv109. Epub 2015 Jul 5.

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OWN - NLM

STAT- Publisher

DA - 20150710

LR - 20150715

IS - 1873-4596 (Electronic)

IS - 0891-5849 (Linking)

DP - 2015 Jul 6

TI - Perfluorooctanoic acid exposure induces endoplasmic reticulum stress in the liver and its effects are ameliorated by 4-phenylbutyrate.

LID - S0891-5849(15)00311-1 [pii]

LID - 10.1016/j.freeradbiomed.2015.06.043 [doi]

AB - Perfluoroalkyl acids (PFAAs) are a group of widely used anthropogenic compounds. As one of the most dominant PFAAs, perfluorooctanoic acid (PFOA) has been suggested to induce hepatotoxicity and several other toxicological effects. However, details on the mechanisms for PFOA-induced hepatotoxicity still need to be elucidated. In this study, we observed the occurrence of endoplasmic reticulum (ER) stress in mouse livers and HepG2 cells after PFOA exposure using several familiar markers for the unfolded protein response (UPR). ER stress in HepG2 cells after PFOA exposure was not significantly influenced by autophagy inhibition or stimulation. The antioxidant defense system was significantly disturbed in mouse livers after PFOA exposure, and reactive oxygen species (ROS) were increased in cells exposed to PFOA for 24h. However, N-acetyl-L-cysteine (NAC) pretreatment did not satisfactorily alleviate the UPR in cells exposed to PFOA even though the increase of ROS was less evident. Furthermore, exposure of HepG2 cells to PFOA in the presence of sodium 4-phenylbutyrate (4-PBA), a chemical chaperone and ER stress inhibitor, suggested that 4-PBA alleviated the UPR and autophagosome accumulation induced by PFOA in cells. In addition, several toxicological effects attributed to PFOA exposure, including cell cycle arrest, proteolytic activity impairment and neutral lipid accumulation, were also improved by 4-PBA co-treatment in cells. In vivo study demonstrated that PFOA-induced lipid metabolism perturbation and liver injury were partially ameliorated by 4-PBA in mice after 28 d exposure. These findings demonstrated that PFOA-induced ER stress leading to UPR might play an important role in PFOA-induced hepatotoxic effects, and chemical chaperone 4-PBA could ameliorate the effects.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150706

TA - Free Radic Biol Med

JT - Free radical biology & medicine

JID - 8709159

OTO - NOTNLM

OT - Hepatotoxicity

OT - Lipid metabolism

OT - Liver injury

OT - Oxidative stress

OT - Sodium 4-phenylbutyrate

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SO - Free Radic Biol Med. 2015 Jul 6. pii: S0891-5849(15)00311-1. doi:  
10.1016/j.freeradbiomed.2015.06.043.

PMID- 26192377

OWN - NLM

STAT- In-Data-Review

DA - 20150808

IS - 1567-7257 (Electronic)

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VI - 34

DP - 2015 Aug

TI - An ST11 clone of *Pasteurella multocida*, widely spread among farmed rabbits in the  
Iberian Peninsula, demonstrates respiratory niche association.

PG - 81-7

LID - 10.1016/j.meegid.2015.07.018 [doi]

LID - S1567-1348(15)00280-4 [pii]

AB - *Pasteurella multocida* is a veterinary pathogen causing diseases with considerable  
economic repercussions in a wide range of animal hosts. In rabbits, *P. multocida*  
infections cause a variety of clinical manifestations including rhinitis,  
pneumonia, septicemia, abscesses, mastitis, and pyometra. In this study, 100 P.



multocida isolates from different commercial rabbit farms located throughout the Iberian Peninsula were molecularly characterized by capsular typing, detection of four virulence-associated genes (tbpA, toxA, hgbB, and pfhA), and multilocus sequence typing (MLST). Rabbit *P. multocida* isolates belonged to three different capsular types: A (47.0%), D (28.0%), and F (25.0%). One group of *P. multocida* isolates of capsular type D and positive for the hgbB gene was significantly associated with the clinical presentation of respiratory disease (OR 5.91; 95%CI, 1.63-21.38). These isolates belonged to same sequence type, ST11, in the *P. multocida* Multi-host MLST database. The ST11 clone also includes isolates from porcine and avian pneumonia. This clonal group of epidemiologically unrelated *P. multocida* isolates could be a virulent clone with some degree of specificity for respiratory disease. These findings could be relevant in the development of vaccines for pasteurellosis prevention, especially respiratory disease.

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LA - eng

PT - Journal Article

DEP - 20150717

PL - Netherlands

TA - Infect Genet Evol

JT - Infection, genetics and evolution : journal of molecular epidemiology and evolutionary genetics in infectious diseases

JID - 101084138

SB - IM

OTO - NOTNLM

OT - MLST

OT - Pasteurella multocida

OT - Pasteurellosis

OT - Rabbit  
 OT - Virulence genes  
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 AID - S1567-1348(15)00280-4 [pii]  
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 PMID- 26212496  
 OWN - NLM  
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 DA - 20150727  
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 IS - 1618-131X (Electronic)  
 IS - 1438-4639 (Linking)  
 DP - 2015 Jul 9  
 TI - Perfluoroalkyl acids in children and their mothers: Association with drinking water and time trends of inner exposures-Results of the Duisburg birth cohort and Bochum cohort studies.  
 LID - S1438-4639(15)00087-5 [pii]  
 LID - 10.1016/j.ijheh.2015.07.001 [doi]  
 AB - BACKGROUND: Perfluoroalkyl acids (PFAAs) are widely distributed in the environment and humans are globally exposed with them. Contaminated drinking water can considerably contribute to the inner exposure levels. OBJECTIVES: We report the results of a human biomonitoring study with mother-child pairs living in two German cities, one city with PFAA contaminated drinking water in the sub mug/l-range (Bochum) and the other one without contamination (Duisburg). Furthermore, we studied time trends of exposure levels within the Duisburg cohort study. METHODS: We measured seven PFAAs (PFOS, PFOA, PFHxS, PFNA, PFBS, PFDeA, PFDoA) in blood samples by high performance liquid chromatography and tandem mass spectrometry. Samples were taken during pregnancy, from umbilical cord blood (2000-2002), 6-7 years (5th follow-up) and 8-10 years after birth (7th follow-up). The consumption of drinking water was recorded by a standardized questionnaire. Statistical analyses were calculated with multiple linear regression models. RESULTS: Children and mothers from Bochum showed higher PFOS and PFOA plasma concentrations than from Duisburg. The median concentrations (mug/l) for children were: PFOS 4.7 vs. 3.3; PFOA 6.0 vs. 3.6mug/l ( $p \leq 0.05$ ). Consumption of  $>0.7$  l (children) and  $>0.9$  l (mothers) drinking water/day was associated with 13-18% higher PFOS, PFOA and PFHxS concentrations in children ( $p \leq 0.01$ ), and 22% higher PFOA in mothers ( $p \leq 0.05$ ). Within the Duisburg cohort, PFAA levels in children peaked in the 5th follow-up study (medians

(µg/l): cord plasma: 2.7 (PFOS); 1.9 (PFOA); 5th follow-up: 3.6 (PFOS); 4.6 (PFOA); 7th follow-up: 3.3 (PFOS); 3.6 (PFOA)). PFOS concentrations in mothers declined from pregnancy to the 5th follow-up (medians: 8.7 vs. 4.0 µg/l).  
CONCLUSION: Residents exposed to PFOS and PFOA through drinking water showed significantly higher PFOS and PFOA concentrations in blood plasma. Although PFAA concentrations in the children slightly decreased from the 5th to the 7th follow-up, we detected increasing exposure trends with increasing age in the 7th follow-up.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150709

TA - Int J Hyg Environ Health

JT - International journal of hygiene and environmental health

JID - 100898843

OTO - NOTNLM

OT - Cohort studies

OT - Drinking water

OT - Human biomonitoring

OT - Mother-child pairs

OT - Perfluoroalkyl acids (PFAAs)

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SO - Int J Hyg Environ Health. 2015 Jul 9. pii: S1438-4639(15)00087-5. doi:  
10.1016/j.ijheh.2015.07.001.

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DA - 20150724  
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IS - 1618-131X (Electronic)  
IS - 1438-4639 (Linking)  
DP - 2015 Jul 9  
TI - Prenatal exposure to perfluoroalkyl substances and children's IQ: The Taiwan  
maternal and infant cohort study.  
LID - S1438-4639(15)00088-7 [pii]  
LID - 10.1016/j.ijheh.2015.07.002 [doi]  
AB - BACKGROUND: Perfluoroalkyl substances (PFASs) are a group of fluorinated organic  
substances that are widely used in consumer products and are often detectable in  
human tissues. Human studies on prenatal exposure to PFASs and neurodevelopment  
in children are few and inconsistent. METHODS: In the Taiwan Maternal and Infant  
Cohort Study, we collected serum samples from pregnant women during the third  
trimester and measured concentrations of 9 PFASs using a high performance liquid  
chromatography system. A subsample of their children was assessed with full scale  
intelligence quotient (FSIQ), verbal IQ (VIQ) and performance IQ (PIQ) at both  
age 5 (n=120) and 8 years (n=120). We used multivariate linear regression models  
to examine prenatal PFAS exposure in relation to IQ scores at each age period.  
RESULTS: Prenatal perfluoroundecanoic acid (PFUnDA) concentrations were inversely  
associated with children's PIQ scores at age 5 years, with an adjusted  
coefficient (beta) of -1.6 (95% confidence interval [CI]: (-3.0, -0.2). When  
children reached 8 years, most of the prenatal PFASs showed inverse association  
with children's FSIQ, VIQ and PIQ scores. Among them, prenatal perfluorononanoic  
acid (PFNA) reached significance. Children with higher prenatal PFNA levels had  
lower VIQ with an adjusted beta of -2.1 (95% CI: -3.9, -0.2). CONCLUSIONS: We  
found two prenatal PFAS exposure, both long-chain PFASs, in association with  
decreased IQ test scores in children. Our findings suggest more studies on  
long-chain PFASs and children's neurodevelopment.

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PT - JOURNAL ARTICLE  
DEP - 20150709  
TA - Int J Hyg Environ Health  
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JID - 100898843  
OTO - NOTNLM  
OT - Children  
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SO - Int J Hyg Environ Health. 2015 Jul 9. pii: S1438-4639(15)00088-7. doi: 10.1016/j.ijheh.2015.07.002.  
  
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DA - 20150527  
IS - 1618-131X (Electronic)  
IS - 1438-4639 (Linking)  
VI - 218  
IP - 5  
DP - 2015 Jul  
TI - Association between perfluoroalkyl substances and reproductive hormones in adolescents and young adults.  
PG - 437-43  
LID - 10.1016/j.ijheh.2015.03.008 [doi]  
LID - S1438-4639(15)00041-3 [pii]  
AB - BACKGROUND: Few studies have explored the association between perfluoroalkyl substances (PFAS) and reproductive hormones in adolescents and young adults. OBJECTIVES: This study aimed to investigate the association of PFAS with reproductive hormones in adolescents and young adults. METHODS: We recruited 540 subjects aged 12-30 years from a 1992 to 2000 mass urine screening population and established a cohort from 2006 to 2008 via invitations by mail or/and telephone. Serum PFAS levels were analyzed with a Waters ACQUITY UPLC system coupled with a Waters Quattro Premier XE triple quadrupole mass spectrometer. Serum reproductive hormone levels were measured by immunoluminometric assay with an Architect random access assay system. PFAS levels were divided into different percentiles according to their detection limits in the multiple regression models to analyze associations between reproductive hormone levels and exposure with PFAS. RESULTS: The adjusted mean serum level of sex hormone-binding globulin (SHBG) decreased significantly in association with the <50th, 50-75, 75-90 and >90th percentile categories of perfluorooctanoic acid (PFOA) compared with a reference category for the females in the 12-17-year-old group. The follicle-stimulating hormone (FSH) levels were significantly decreased in association with the different percentile categories of perfluorooctane sulfonate (PFOS) in the male 12-17-year-old group and the different percentile categories of perfluoroundecanoic acid (PFUA) in the female 12-17-year-old group. The serum FSH levels in the females aged 12-17 were also decreased in association with the different percentile categories of PFUA. On the other hand, there was a significantly negative association between the different percentile categories of PFOS and the serum testosterone level among the female 12-17-year-old group. CONCLUSIONS: We found that the serum concentrations of PFOA, PFOS, and PFUA were negatively associated with the serum levels of SHBG, FSH, and testosterone in the young Taiwanese population and that these effects were the strongest in the females aged 12-17. Further studies are needed to determine whether these associations are causal.  
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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150326

PL - Germany

TA - Int J Hyg Environ Health

JT - International journal of hygiene and environmental health

JID - 100898843

SB - IM

OTO - NOTNLM  
 OT - Adolescent  
 OT - Perfluoroalkyl substances  
 OT - Reproductive hormone  
 OT - Young adults  
 EDAT- 2015/04/30 06:00  
 MHDA- 2015/04/30 06:00  
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 PHST- 2014/11/12 [received]  
 PHST- 2015/03/16 [revised]  
 PHST- 2015/03/17 [accepted]  
 PHST- 2015/03/26 [aheadofprint]  
 AID - S1438-4639(15)00041-3 [pii]  
 AID - 10.1016/j.ijheh.2015.03.008 [doi]  
 PST - ppublish  
 SO - Int J Hyg Environ Health. 2015 Jul;218(5):437-43. doi:  
 10.1016/j.ijheh.2015.03.008. Epub 2015 Mar 26.  
  
 PMID- 25941995  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150729  
 IS - 1930-8264 (Electronic)  
 IS - 1930-8264 (Linking)  
 VI - 105  
 IP - 4  
 DP - 2015 Jul  
 TI - A Randomized Controlled Trial of Custom Foot Orthoses for the Treatment of  
 Plantar Heel Pain.  
 PG - 281-94  
 LID - 10.7547/13-122.1 [doi]  
 AB - BACKGROUND: Up to 10% of people will experience heel pain. The purpose of this  
 prospective, double-blind, randomized clinical trial was to compare custom foot  
 orthoses (CFO), prefabricated foot orthoses (PFO), and sham insole treatment for  
 plantar fasciitis. METHODS: Seventy-seven patients with plantar fasciitis for  
 less than 1 year were included. Outcome measures included first step and end of  
 day pain, Revised Foot Function Index short form (FFI-R), 36-Item Short Form  
 Health Survey (SF-36), activity monitoring, balance, and gait analysis. RESULTS:  
 The CFO group had significantly improved total FFI-R scores (77.4 versus 57.2; P  
 = .03) without group differences for FFI-R pain, SF-36, and morning or evening  
 pain. The PFO and CFO groups reported significantly lower morning and evening  
 pain. For activity, the CFO group demonstrated significantly longer episodes of  
 walking over the sham (P = .019) and PFO (P = .03) groups, with a 125% increase  
 for CFOs, 22% PFOs, and 0.2% sham. Postural transition duration (P = .02) and  
 balance (P = .05) improved for the CFO group. There were no gait differences. The  
 CFO group reported significantly less stretching and ice use at 3 months.  
 CONCLUSIONS: The CFO group demonstrated 5.6-fold greater improvements in  
 spontaneous physical activity versus the PFO and sham groups. All three groups



improved in morning pain after treatment that included standardized athletic shoes, stretching, and ice. The CFO changes may have been moderated by decreased stretching and ice use after 3 months. These findings suggest that more objective measures, such as spontaneous physical activity improvement, may be more sensitive and specific for detecting improved weightbearing function than traditional clinical outcome measures, such as pain and disease-specific quality of life.

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LA - eng

PT - Journal Article

DEP - 20150505

PL - United States

TA - J Am Podiatr Med Assoc

JT - Journal of the American Podiatric Medical Association

JID - 8501423

SB - IM

EDAT- 2015/05/06 06:00

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AID - 10.7547/13-122.1 [doi]

PST - ppublish

SO - J Am Podiatr Med Assoc. 2015 Jul;105(4):281-94. doi: 10.7547/13-122.1. Epub 2015 May 5.

PMID- 26178269

OWN - NLM

STAT- Publisher

DA - 20150716

LR - 20150717

IS - 1099-1263 (Electronic)

IS - 0260-437X (Linking)

DP - 2015 Jul 15

TI - Protein profiles of cardiomyocyte differentiation in murine embryonic stem cells exposed to perfluorooctane sulfonate.

LID - 10.1002/jat.3207 [doi]

AB - Perfluorooctane sulfonate (PFOS) is a persistent organic contaminant that may affect diverse systems in animals and humans, including the cardiovascular system. However, little is known about the mechanism by which it affects the

biological systems. Herein, we used embryonic stem cell test procedure as a tool to assess the developmental cardiotoxicity of PFOS. The differentially expressed proteins were identified by quantitative proteomics that combines the stable isotope labeling of amino acids with high-performance liquid chromatography-electrospray ionization tandem mass spectrometry. Results of the embryonic stem cell test procedure suggested that PFOS was a weak embryotoxic chemical. Nevertheless, a few marker proteins related to cardiovascular development (Brachyury, GATA4, MEF2C, alpha-actinin) were significantly reduced by exposure to PFOS. In total, 176 differential proteins were identified by proteomics analysis, of which 67 were upregulated and 109 were downregulated. Gene ontology annotation classified these proteins into 13 groups by molecular functions, 12 groups by cellular locations and 10 groups by biological processes. Most proteins were mainly relevant to either catalytic activity (25.6%), nucleus localization (28.9%) or to cellular component organization (19.8%). Pathway analysis revealed that 32 signaling pathways were affected, particularly these involved in metabolism. Changes in five proteins, including L-threonine dehydrogenase, X-ray repair cross-complementing 5, superoxide dismutase 2, and DNA methyltransferase 3b and 3a were confirmed by Western blotting, suggesting the reliability of the technique. These results revealed potential new targets of PFOS on the developmental cardiovascular system. Copyright (c) 2015 John Wiley & Sons, Ltd.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150715

TA - J Appl Toxicol

JT - Journal of applied toxicology : JAT

JID - 8109495

OTO - NOTNLM  
OT - cardiomyocyte  
OT - embryonic stem cell test (EST)  
OT - embryotoxicity  
OT - perfluorooctane sulfonate (PFOS)  
OT - quantitative proteomics  
EDAT- 2015/07/17 06:00  
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PHST- 2015/06/03 [revised]  
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AID - 10.1002/jat.3207 [doi]  
PST - aheadofprint  
SO - J Appl Toxicol. 2015 Jul 15. doi: 10.1002/jat.3207.

PMID- 26165890  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150713  
IS - 1948-8270 (Electronic)  
IS - 1948-8270 (Linking)  
VI - 22  
IP - 3  
DP - 2015 Jul  
TI - Ultrasound-guided Percutaneous Needle Aspiration by Pulmonologists: A Study of Factors With Impact on Procedural Yield and Complications.  
PG - 204-8  
LID - 10.1097/LBR.0000000000000175 [doi]  
AB - BACKGROUND: The availability of portable ultrasound (US) guidance has led to usage by subspecialists outside of radiology. Several subspecialties now perform percutaneous fine-needle aspiration (PFNA) for lesions relevant to their expertise. This is a study of US-guided PFNA performed by interventional pulmonologists at a single institution. METHODS: We retrospectively reviewed serial US-guided PFNAs performed at an institution with the goals of defining yield, factors relating to yield, and complication rates. RESULTS: A total of 111 consecutive lesions were evaluated and 109 biopsied during the study period. Diagnosis was established in 81% of cases (90/109), with a total complication rate of 15% but only 1 case of a need for a higher level of care. Factors associated with increased diagnostic yield were suspicion of malignancy, increased size, and pleural adhesions (lack of pleural sliding). The presence of pleural sliding was associated with increased pneumothorax and decreased yield. CONCLUSIONS: US-guided PFNA is a valuable tool for the interventional pulmonologist. Both size and pleural sliding have an impact on diagnostic yield.  
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FAU - Bartter, Thaddeus  
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 LA - eng  
 PT - Journal Article  
 PL - United States  
 TA - J Bronchology Interv Pulmonol  
 JT - Journal of bronchology & interventional pulmonology  
 JID - 101496866  
 SB - IM  
 EDAT- 2015/07/15 06:00  
 MHDA- 2015/07/15 06:00  
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 AID - 10.1097/LBR.0000000000000175 [doi]  
 AID - 01436970-201507000-00004 [pii]  
 PST - ppublish  
 SO - J Bronchology Interv Pulmonol. 2015 Jul;22(3):204-8. doi:  
 10.1097/LBR.0000000000000175.  
  
 PMID- 26070818  
 OWN - NLM  
 STAT- In-Process  
 DA - 20150616  
 IS - 1873-3778 (Electronic)  
 IS - 0021-9673 (Linking)  
 VI - 1404  
 DP - 2015 Jul 24  
 TI - Determination of fluorotelomer alcohols and their degradation products in  
 biosolids-amended soils and plants using ultra-high performance liquid  
 chromatography tandem mass spectrometry.  
 PG - 72-80  
 LID - 10.1016/j.chroma.2015.05.063 [doi]  
 LID - S0021-9673(15)00786-4 [pii]  
 AB - Degradation of fluorotelomer alcohols (FTOHs) was recognized as an additional  
 source of perfluorocarboxylic acids (PFCAs). Quantification of FTOHs and their  
 degradation products can help shed light on the sources and fates of PFCAs in the  
 environment. In this study, an analytical method was developed for the  
 determination of 6:2 and 8:2 FTOHs, and their degradation products of poly- and  
 perfluorinated acids, including fluorotelomer saturated and unsaturated  
 carboxylic acids (FTCAs and FTUCAs), secondary polyfluorinated alcohols and PFCAs  
 in biosolids-amended soils and plants using ultra-high performance liquid  
 chromatography tandem mass spectrometry (UPLC-MS/MS). The extract efficiencies of  
 different methods including ethyl acetate and methanol (MeOH) for FTOHs and  
 acetonitrile, MeOH, methyl tert-butyl ether (MTBE), NaOH-MeOH and NaOH-MTBE for  
 poly- and perfluorinated acids were tested. The results showed that 6:2 and 8:2  
 FTOHs and their degradation products could be simultaneously and satisfactorily  
 extracted by MeOH, cleaned up by Envi-Carb graphitized carbon and solid phase  
 extraction, respectively, and determined by UPLC-MS/MS separately. NaOH in the  
 extractant caused the conversion of 6:2 FTCA and 8:2 FTCA into the corresponding

FTUCAs. The selected methods have matrix recoveries ranged from 52% to 102%, and detection limits of 0.01-0.46ng/g dry weight for FTOHs and their degradation products in soil and plant. The optimized method was applied successfully to quantify FTOHs and their degradation products in two biosolids-amended soils and plants. The total concentrations of FTOHs in the soils were 44.1+/-5.8 and 82.6+/-7.1ng/g, and in plants tissues 3.58+/-0.25 and 8.33+/-0.66ng/g. The total concentrations of poly- and perfluorinated acids in the soils were 168.0+/-13.2 and 349.6+/-11.2ng/g, and in plants tissues 78.0+/-6.4 and 75.5+/-5.3ng/g.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150604

PL - Netherlands

TA - J Chromatogr A

JT - Journal of chromatography. A  
 JID - 9318488  
 SB - IM  
 OTO - NOTNLM  
 OT - Biosolids-amended soil  
 OT - Degradation products  
 OT - FTOHs  
 OT - Plant  
 OT - UPLC-MS/MS  
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 AID - S0021-9673(15)00786-4 [pii]  
 AID - 10.1016/j.chroma.2015.05.063 [doi]  
 PST - ppublish  
 SO - J Chromatogr A. 2015 Jul 24;1404:72-80. doi: 10.1016/j.chroma.2015.05.063. Epub  
 2015 Jun 4.  
  
 PMID- 26195039  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150803  
 IS - 1873-3778 (Electronic)  
 IS - 0021-9673 (Linking)  
 VI - 1408  
 DP - 2015 Aug 21  
 TI - Ion-pair reversed phase liquid chromatography with ultraviolet detection for  
 analysis of ultraviolet transparent cations.  
 PG - 261-6  
 LID - 10.1016/j.chroma.2015.07.026 [doi]  
 LID - S0021-9673(15)00977-2 [pii]  
 AB - This paper describes the use of an anionic ion-pair reagent (IPR) to improve the  
 ultraviolet (UV) detection and hydrophobic retention of polar and UV transparent  
 cations. Anionic IPR added to the mobile phase forms an ion-pair with cations.  
 Formation of the ion-pair causes a redshift in the absorption wavelength, making it  
 possible for direct UV detection of UV-inactive cations. The ion-pairs with  
 increased hydrophobicity were separated by reversed phase liquid chromatography  
 (RPLC). Different perfluorinated carboxylic acids (trifluoroacetic acid,  
 heptafluorobutyric acid, nonafluoropentanoic acid) were evaluated as IPR in the  
 separation and detection of the common cations sodium, ammonium and  
 Tris(hydroxymethyl)aminomethane (Tris). The effects of the IPR type and  
 concentration on separation and detection have been investigated to understand  
 the separation and detection mechanisms. The optimal separation and detection  
 conditions were attained with mobile phase containing 0.1% nonafluoropentanoic

acid and with the UV detection at 210nm. UV detection and charged aerosol detection (CAD) were compared in the quantitation of the cations. The limit of quantitation (LOQ) of sodium and Tris with UV detection is comparable to that by CAD. The LOQ of ammonium with UV detection (1ppm or 3ng) is about 20-fold lower than that (20ppm or 60ng) by CAD. The RPLC-UV method was used to monitor ammonium clearance during ultrafiltration and diafiltration in the manufacturing of biopharmaceutical drug substance.

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LA - eng

PT - Journal Article

DEP - 20150713

PL - Netherlands

TA - J Chromatogr A

JT - Journal of chromatography. A

JID - 9318488

SB - IM

OTO - NOTNLM

OT - Cations

OT - Improve UV detection

OT - Ion-pair RPLC

EDAT- 2015/07/22 06:00

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 PHST- 2015/07/13 [aheadofprint]  
 AID - S0021-9673(15)00977-2 [pii]  
 AID - 10.1016/j.chroma.2015.07.026 [doi]  
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 SO - J Chromatogr A. 2015 Aug 21;1408:261-6. doi: 10.1016/j.chroma.2015.07.026. Epub 2015 Jul 13.

PMID- 26210101  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150812  
 IS - 1095-7103 (Electronic)  
 IS - 0021-9797 (Linking)  
 VI - 458  
 DP - 2015 Nov 15  
 TI - Modification of fluororous substrates with oligo(ethylene glycol) via "click" chemistry for long-term resistance of cell adhesion.  
 PG - 112-8  
 LID - 10.1016/j.jcis.2015.07.033 [doi]  
 LID - S0021-9797(15)30052-7 [pii]  
 AB - In this work perfluorinated substrates fabricated from SiO<sub>2</sub> glass slides are modified with oligo(ethylene glycol) (OEG) units for long-term resistance of cell adhesion purposes, based on fluororous interactions and click chemistry. Specifically, fluororous substrates, prepared by treatment of glass slides with 1H, 1H, 2H, 2H-perfluorodecyltrimethoxysilane (FAS17), were coated with ethynyl-OEG-C8F17, followed by covalent attachment of an azido-OEG via copper-catalyzed azide-alkyne cycloaddition (CuAAC) "click" reaction. We demonstrate that the resultant surface avoid fibrinogen adsorption and resisted cell adhesion for over 14days. X-ray photoemission spectroscopy (XPS) analysis and contact angle goniometry measurements confirm the presence of the OEG molecules on the fluororous substrates. Bright field optical images show total absence of 3T3 fibroblast cells on the OEG modified fluorinated substrate for 1 and 5days, and a remarkably decrease of cell adhesion at 14days.  
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LA - eng

PT - Journal Article

DEP - 20150715

PL - United States

TA - J Colloid Interface Sci

JT - Journal of colloid and interface science

JID - 0043125

SB - IM

OTO - NOTNLM

OT - Cell adhesion resistance

OT - Click reaction

OT - Fluorinated substrate

OT - Fluorine-fluorine interaction

OT - OEG

OT - Protein resistance  
EDAT- 2015/07/27 06:00  
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PHST- 2015/07/11 [revised]  
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AID - S0021-9797(15)30052-7 [pii]  
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DA - 20150817  
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IS - 1873-3336 (Electronic)  
IS - 0304-3894 (Linking)  
VI - 299  
DP - 2015 Jul 31  
TI - Occurrence, fluxes and sources of perfluoroalkyl substances with isomer analysis  
in the snow of northern China.  
PG - 639-646  
LID - S0304-3894(15)00611-1 [pii]  
LID - 10.1016/j.jhazmat.2015.07.074 [doi]  
AB - In this study, perfluoroalkyl substances (PFASs) and the isomers of  
perfluorooctanoate (PFOA) and perfluorooctanesulfonate (PFOS) were analyzed in  
fresh snow samples collected from 19 cities in northern China, 2013. The levels  
of total PFASs in the snow samples were 33.5-229ng/L, suggesting heavy  
atmospheric pollution of PFASs in northern China. PFOA (9.08-107ng/L), PFOS  
(3.52-54.3ng/L), perfluoroheptanoate (PFHpA) (3.66-44.8ng/L), and  
perfluorohexanoate (PFHxA) (3.21-23.6ng/L) were predominant with a summed  
contribution of 82% to the total PFASs. The particulate matters (PMs) associated  
PFASs contributed 21.5-56.2% to the total PFASs in the snow, suggesting PMs are  
vital for the transport and deposition of airborne PFASs. Partitioning of PFASs  
between PM and dissolved phases was dependent on the carbon chain length and end  
functional groups. Isomer profiles of PFOA and PFOS in the snow were in agreement  
with the signature of the historical 3M electrochemical fluorination (ECF)  
products, suggesting that the ECF products were still produced and used in China.  
Further source analysis showed that the airborne PFASs in urban area were mainly  
due to direct release rather than degradation of their precursors.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150731

TA - J Hazard Mater

JT - Journal of hazardous materials

JID - 9422688

OTO - NOTNLM

OT - Isomers

OT - PFOA

OT - PFOS

OT - Snow

OT - Sources

EDAT- 2015/08/19 06:00

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AID - 10.1016/j.jhazmat.2015.07.074 [doi]

PST - aheadofprint

SO - J Hazard Mater. 2015 Jul 31;299:639-646. doi: 10.1016/j.jhazmat.2015.07.074.

PMID- 26181512

OWN - NLM

STAT- Publisher

DA - 20150716

LR - 20150717

IS - 1547-6901 (Electronic)

IS - 1547-691X (Linking)

DP - 2015 Jul 16

TI - Antibody response to booster vaccination with tetanus and diphtheria in adults exposed to perfluorinated alkylates.

PG - 1-4

AB - Recent studies suggest that exposure to perfluorinated alkylate substances (PFASs) may induce immunosuppression in humans and animal models. In this exploratory study, 12 healthy adult volunteers were recruited. With each subject, serum-PFAS concentrations were measured and their antibody responses prospectively followed for 30 days after a booster vaccination with diphtheria and tetanus. The results indicated that serum-PFAS concentrations were positively correlated and positively associated with age and male sex. The specific antibody concentrations in serum were increased from Day 4 to Day 10 post-booster, after which a constant concentration was reached. Serum PFAS concentrations showed significant negative associations with the rate of increase in the antibody responses. Interestingly, this effect was particularly strong for the longer-chain PFASs. All significant associations remained significant after adjustment for sex and age. Although the study involved a small number of subjects, these findings of a PFAS-associated reduction of the early humoral immune response to booster vaccination in healthy adults supported previous findings of PFAS immunosuppression in larger cohorts. Furthermore, the results suggested that cellular mechanisms right after antigen exposure should be investigated more closely to identify possible mechanisms of immunosuppression from PFAS.

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FAU - Heilmann, Carsten

AU - Heilmann C

LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150716

TA - J Immunotoxicol

JT - Journal of immunotoxicology

JID - 101201960

OTO - NOTNLM

OT - Antibodies

OT - immunotoxicity

OT - perfluorinated alkylate substances

OT - prospective study

OT - vaccinations

EDAT- 2015/07/17 06:00

MHDA- 2015/07/17 06:00  
CRDT- 2015/07/17 06:00  
AID - 10.3109/1547691X.2015.1067259 [doi]  
PST - aheadofprint  
SO - J Immunotoxicol. 2015 Jul 16:1-4.

PMID- 26076067  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150718  
IS - 1520-6904 (Electronic)  
IS - 0022-3263 (Linking)  
VI - 80  
IP - 14  
DP - 2015 Jul 17  
TI - Micelle Formation in Liquid Ammonia.  
PG - 7033-9  
LID - 10.1021/acs.joc.5b00830 [doi]  
AB - Perfluorinated long chain alkyl amides aggregate in liquid ammonia with increasing concentration which reflects micelle-type formation based on changes in <sup>19</sup>F NMR chemical shifts. The critical micelle concentrations (cmc) decrease with increasing chain length and give Kleven parameters A = 0.18 and B = 0.19. The micelles catalyze the ammonolysis of esters in liquid ammonia. The corresponding perfluorinated long chain alkyl carboxylates form ion pairs in liquid ammonia, but the equilibrium dissociation constants indicate favorable interactions between the chains in addition to the electrostatic forces. These perfluorinated carboxylates form micelles in aqueous solution, and their cmc's generate a Kleven B-value = 0.52 compared with 0.30 for the analogous alkyl carboxylates. The differences in hydrophobicity of CH<sub>2</sub> and CF<sub>2</sub> units in water and liquid ammonia are discussed, as is the possible relevance to life forms in liquid ammonia.

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LA - eng  
PT - Journal Article  
DEP - 20150630  
PL - United States  
TA - J Org Chem

JT - The Journal of organic chemistry

JID - 2985193R

SB - IM

EDAT- 2015/06/16 06:00

MHDA- 2015/06/16 06:00

CRDT- 2015/06/16 06:00

PHST- 2015/06/30 [aheadofprint]

AID - 10.1021/acs.joc.5b00830 [doi]

PST - ppublish

SO - J Org Chem. 2015 Jul 17;80(14):7033-9. doi: 10.1021/acs.joc.5b00830. Epub 2015 Jun 30.

PMID- 26197959

OWN - NLM

STAT- Publisher

DA - 20150722

LR - 20150723

IS - 1436-2023 (Electronic)

IS - 0949-2658 (Linking)

DP - 2015 Jul 22

TI - Do PFNA devices and Intertan nails both have the same effects in the treatment of trochanteric fractures? A prospective clinical study.

AB - **OBJECTIVE:** To clinically and radiologically compare third-generation intramedullary nails used in the treatment of trochanteric hip fractures and to determine their efficacy. **MATERIALS AND METHODS:** Seventy-five of 88 patients admitted to our hospital with trochanteric fractures were enrolled in the study; 43 were treated with PFNA devices and 32 with Intertan nails. The amount of compression applied during the procedure, duration of the procedure, amount of subsequent shortening in the proximal femoral area, subsequent backup of proximal screws, and changes in the tip-apex and tip-cortex distances were compared between groups. The postoperative change in the varus angle of the proximal femur and times to mobilization, full weight bearing, and fracture union were also evaluated. **RESULTS:** On early postoperative radiographs, the tip-apex distance was  $\leq 25$  mm in 86 % of patients in the PFNA group and 96.9 % of those in the Intertan group. Twelve months postoperatively, the tip-apex distance did not differ between groups. No cut-out of the screws into the coxofemoral joint was observed. Fracture healing was achieved in all patients. At 12 months postoperatively, the rates of proximal screw backup, proximal femoral shortening, and decrease in the varus angle of the proximal femur were significantly higher in the PFNA group than in the Intertan group. **CONCLUSIONS:** Trochanteric fractures may be treated effectively with PFNA devices or Intertan nails. During the healing period, the rates of reverse displacement of the proximal screw, shortening of the proximal femur, and decrease in the varus angle of the proximal femur were significantly higher in the PFNA group than in the Intertan group. Surgical technique, implant positioning, and the choice of implant play roles in the successful treatment of trochanteric fractures. **LEVEL OF EVIDENCE:** Level 1, prospective, prognostic study.

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 LA - ENG  
 PT - JOURNAL ARTICLE  
 DEP - 20150722  
 TA - J Orthop Sci  
 JT - Journal of orthopaedic science : official journal of the Japanese Orthopaedic Association  
 JID - 9604934  
 EDAT- 2015/07/23 06:00  
 MHDA- 2015/07/23 06:00  
 CRDT- 2015/07/23 06:00  
 PHST- 2014/12/20 [received]  
 PHST- 2015/07/02 [accepted]  
 PHST- 2015/07/22 [aheadofprint]  
 AID - 10.1007/s00776-015-0750-4 [doi]  
 PST - aheadofprint  
 SO - J Orthop Sci. 2015 Jul 22.  
  
 PMID- 26222276  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150729  
 LR - 20150730  
 IS - 1873-264X (Electronic)  
 IS - 0731-7085 (Linking)  
 VI - 115  
 DP - 2015 Jul 17  
 TI - Direct tandem mass spectrometric analysis of amino acids in plasma using fluorous derivatization and monolithic solid-phase purification.  
 PG - 201-207  
 LID - S0731-7085(15)30062-5 [pii]  
 LID - 10.1016/j.jpba.2015.07.008 [doi]  
 AB - In this study, we developed a novel direct tandem mass spectrometric method for rapid and accurate analysis of amino acids utilizing a fluorous derivatization and purification technique. Amino acids were perfluoroalkylated with 2H,2H,3H,3H-perfluoroundecan-1-ol in the presence of 2-picoline borane via reductive amination. The derivatives were purified by perfluoroalkyl-modified silica-based monolithic solid-phase extraction (monolithic F-SPE), and directly analyzed by tandem mass spectrometry using electrospray ionization without liquid chromatographic separation. The perfluoroalkyl derivatives could be sufficiently

distinguished from non-fluororous compounds, i.e. the biological matrix, due to their fluororous interaction. Thus, rapid and accurate determination of amino acids was accomplished. The method was validated with human plasma samples and applied to the analysis of amino acids in the plasma of mice with maple syrup urine disease or phenylketonuria.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150717

TA - J Pharm Biomed Anal

JT - Journal of pharmaceutical and biomedical analysis

JID - 8309336

OTO - NOTNLM

OT - Amino acids

OT - Direct tandem mass spectrometric analysis

OT - Fluororous derivatization

OT - Monolithic fluororous solid-phase extraction

EDAT- 2015/07/30 06:00

MHDA- 2015/07/30 06:00

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PHST- 2015/05/07 [received]

PHST- 2015/07/09 [revised]

PHST- 2015/07/10 [accepted]

AID - S0731-7085(15)30062-5 [pii]



AID - 10.1016/j.jpba.2015.07.008 [doi]  
 PST - aheadofprint  
 SO - J Pharm Biomed Anal. 2015 Jul 17;115:201-207. doi: 10.1016/j.jpba.2015.07.008.  
  
 PMID- 26095172  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150817  
 LR - 20150817  
 IS - 1472-765X (Electronic)  
 IS - 0266-8254 (Linking)  
 VI - 61  
 IP - 3  
 DP - 2015 Sep  
 TI - Development of a novel multiplex PCR assay for rapid detection of virulence associated genes of *Pasteurella multocida* from pigs.  
 PG - 293-298  
 LID - 10.1111/lam.12453 [doi]  
 AB - As the pathogenicity of *Pasteurella multocida* is associated with various virulence factors (VFs), the aim of the study was to develop a novel multiplex PCR (m-PCR) assay for the rapid detection of important virulence associated genes (VAGs) of *P. multocida* isolates from pigs. The target recognized VFs used in the study were diverse adhesins (ptfA and pfhA), toxins (toxA), siderophores (tonB and hgbA), sialidases (nanB, nanH) and outer membrane proteins (ompA, ompH, oma87 and plpB). The primers for the genes encoding these VFs were designed by primer3 software (<http://bioinfo.ut.ee/primer3-0.4.0/>) using gene sequences available in Genbank. The detection limit of the developed assay was 102 CFU ml<sup>-1</sup>. The m-PCR did not produce any nonspecific amplification products when tested against *Bordetella bronchiseptica* which also commonly infects pigs. We applied m-PCR to the field samples, and the results obtained were the same as the single PCR results. The developed assay would be very useful for veterinary diagnostic laboratories and for others interested in the rapid virulence profiling of porcine *P. multocida* isolates circulating in the piggeries. SIGNIFICANCE AND IMPACT OF THE STUDY: The study reports the development and evaluation of a novel multiplex PCR assay for the rapid detection of 11 important VAGs of *Pasteurella multocida* isolates from pigs. Rapid and simultaneous detection of recognized VFs of the organism are essential to know the virulo-types of *P. multocida* isolates circulating in the piggeries. The developed novel assay will be very useful for the rapid detection of VAGs of *P. multocida* isolates from pigs.  
 CI - (c) 2015 The Society for Applied Microbiology.  
 FAU - Rajkhowa, S  
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 AD - National Research Centre on Pig, Indian Council of Agricultural Research, Guwahati, Assam, India.  
 LA - ENG  
 SI - GENBANK/U50907  
 SI - GENBANK/U60439  
 SI - GENBANK/NC\_017027.1

SI - GENBANK/EU408787.1  
 SI - GENBANK/AY644678.1  
 SI - GENBANK/AY035342  
 SI - GENBANK/AE006158.1  
 SI - GENBANK/NC\_016808.1  
 SI - GENBANK/AF274868  
 SI - GENBANK/AF274869  
 SI - GENBANK/AF240778  
 PT - JOURNAL ARTICLE  
 DEP - 20150707  
 TA - Lett Appl Microbiol  
 JT - Letters in applied microbiology  
 JID - 8510094  
 OTO - NOTNLM  
 OT - Pasteurella multocida  
 OT - multiplex PCR  
 OT - porcine  
 OT - rapid detection  
 OT - virulence associated genes  
 EDAT- 2015/06/23 06:00  
 MHDA- 2015/06/23 06:00  
 CRDT- 2015/06/23 06:00  
 PHST- 2015/04/04 [received]  
 PHST- 2015/05/18 [revised]  
 PHST- 2015/06/02 [accepted]  
 PHST- 2015/07/07 [aheadofprint]  
 AID - 10.1111/lam.12453 [doi]  
 PST - ppublish  
 SO - Lett Appl Microbiol. 2015 Sep;61(3):293-298. doi: 10.1111/lam.12453. Epub 2015 Jul 7.  
  
 PMID- 26028170  
 OWN - NLM  
 STAT- In-Process  
 DA - 20150615  
 IS - 1879-3363 (Electronic)  
 IS - 0025-326X (Linking)  
 VI - 96  
 IP - 1-2  
 DP - 2015 Jul 15  
 TI - Spatial distribution and fate of perfluoroalkyl substances in sediments from the Pearl River Estuary, South China.  
 PG - 226-34  
 LID - 10.1016/j.marpolbul.2015.05.022 [doi]  
 LID - S0025-326X(15)00279-9 [pii]  
 AB - In this study, 54 sediment samples were collected from the Pearl River Estuary (PRE) in Southern China to study the spatial distribution and patterns of PFASs in this region. PFAS concentrations in the sediment samples ranged from nd (below

detection limit) to 2.41 ng g<sup>(-1)</sup> dw (dry weight) with an average value of 0.79 ng g<sup>(-1)</sup> dw. PFAS concentrations were higher at the nearshore sampling sites than in the others. Perfluorobutanesulfonate (PFBS) and perfluorohexanesulfonate (PFHxS) were the two dominant compounds among the target PFASs, which may be due to their production and use as PFOS substitutes in the Pearl River Delta (PRD) areas. Significant linear relationships were found between total PFAS concentrations and total organic carbon (TOC) ( $R=0.30$ ,  $p<0.05$ ). The preliminary environmental risk assessment indicated that PFOS and PFOA in the regional sediments posed no significant ecological risk to the benthic organisms at present levels.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150528

PL - England

TA - Mar Pollut Bull

JT - Marine pollution bulletin  
 JID - 0260231  
 SB - IM  
 OTO - NOTNLM  
 OT - PFASs  
 OT - Pearl River Estuary  
 OT - Risk assessment  
 OT - Sediment  
 EDAT- 2015/06/02 06:00  
 MHDA- 2015/06/02 06:00  
 CRDT- 2015/06/02 06:00  
 PHST- 2014/10/22 [received]  
 PHST- 2015/05/12 [revised]  
 PHST- 2015/05/12 [accepted]  
 PHST- 2015/05/28 [aheadofprint]  
 AID - S0025-326X(15)00279-9 [pii]  
 AID - 10.1016/j.marpolbul.2015.05.022 [doi]  
 PST - ppublish  
 SO - Mar Pollut Bull. 2015 Jul 15;96(1-2):226-34. doi:  
 10.1016/j.marpolbul.2015.05.022. Epub 2015 May 28.  
  
 PMID- 26158308  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150803  
 IS - 1543-8392 (Electronic)  
 IS - 1543-8384 (Linking)  
 VI - 12  
 IP - 8  
 DP - 2015 Aug 3  
 TI - Antiangiogenic and Anticancer Properties of Bifunctional Ruthenium(II)-p-Cymene  
 Complexes: Influence of Pendant Perfluorous Chains.  
 PG - 3089-96  
 LID - 10.1021/acs.molpharmaceut.5b00417 [doi]  
 AB - Two bifunctional ruthenium(II)-p-cymene complexes with perfluorinated side  
 chains, attached via pyridine ligands, have been evaluated in a series of in  
 vitro and in vivo assays. Their effects on human endothelial (ECRF24 and HUVEC)  
 cells, noncancerous human embryonic kidney (HEK-293) cells, and various human  
 tumor cells were investigated. The complex with the shorter chain, 1, inhibits  
 the proliferation of the tumor cell lines and ECRF24, whereas 2 selectively  
 inhibits ECRF24 and HUVEC proliferation. Neither inhibits the migration of ECRF24  
 cells whereas both compounds inhibit sprout formation in HUVEC cells. Using three  
 preclinical models, i.e., vasculature formation in the chorioallantoic membrane  
 (CAM) of the chicken embryo, human A2780 ovarian carcinoma tumors xenografted on  
 the CAM, and human LS174T colorectal adenocarcinoma tumors grown in athymic mice,  
 the angiostatic and anticancer activities of these two complexes were studied.  
 Overall, 1 inhibited tumor growth predominantly through an anticancer effect  
 whereas 2 inhibited tumor growth predominately via an antiangiogenic mechanism.

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LA - eng  
PT - Journal Article  
DEP - 20150721  
PL - United States  
TA - Mol Pharm  
JT - Molecular pharmaceuticals  
JID - 101197791  
SB - IM  
OTO - NOTNLM  
OT - CAM model  
OT - antiangiogenesis  
OT - bioorganometallic chemistry  
OT - colorectal adenocarcinoma  
OT - fluorine chemistry  
OT - ovarian carcinoma  
OT - ruthenium(II)-arene complexes  
EDAT- 2015/07/15 06:00  
MHDA- 2015/07/15 06:00  
CRDT- 2015/07/10 06:00  
PHST- 2015/07/21 [aheadofprint]

AID - 10.1021/acs.molpharmaceut.5b00417 [doi]  
 PST - ppublish  
 SO - Mol Pharm. 2015 Aug 3;12(8):3089-96. doi: 10.1021/acs.molpharmaceut.5b00417. Epub 2015 Jul 21.  
  
 PMID- 26140545  
 OWN - NLM  
 STAT- In-Data-Review  
 DA - 20150722  
 IS - 1477-0539 (Electronic)  
 IS - 1477-0520 (Linking)  
 VI - 13  
 IP - 30  
 DP - 2015 Jul 22  
 TI - Efficient one-pot synthesis of 5-perfluoroalkylpyrazoles by cyclization of hydrazone dianions.  
 PG - 8277-90  
 LID - 10.1039/c5ob01151e [doi]  
 AB - A highly selective and efficient method for the synthesis of 5-trifluoromethylated and 5-perfluoroalkylated pyrazoles has been developed which relies on the cyclization of hydrazine dianions with ethyl perfluorocarboxylates. The pyrazoles prepared were evaluated as potential inhibitors of alkaline phosphatases, namely human tissue non-specific alkaline phosphatase (h-TNAP) and tissue specific intestinal alkaline phosphatase (IAP). Most pyrazole derivatives inhibited h-IAP more markedly than h-TNAP and had minor effects on nucleotide pyrophosphatase/phosphodiesterases. Therefore, the compounds appear as potential selective inhibitors of h-IAP.  
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 FAU - Langer, Peter  
 AU - Langer P  
 LA - eng  
 PT - Journal Article  
 PL - England

TA - Org Biomol Chem  
JT - Organic & biomolecular chemistry  
JID - 101154995  
SB - IM  
EDAT- 2015/07/04 06:00  
MHDA- 2015/07/04 06:00  
CRDT- 2015/07/04 06:00  
AID - 10.1039/c5ob01151e [doi]  
PST - ppublish  
SO - Org Biomol Chem. 2015 Jul 22;13(30):8277-90. doi: 10.1039/c5ob01151e.

PMID- 26090551  
OWN - NLM  
STAT- In-Data-Review  
DA - 20150703  
IS - 1523-7052 (Electronic)  
IS - 1523-7052 (Linking)  
VI - 17  
IP - 13  
DP - 2015 Jul 2  
TI - Mild and Efficient One-Pot Synthesis of 2-(Perfluoroalkyl)indoles by Means of Sequential Michael-Type Addition and Pd(II)-Catalyzed Cross-Dehydrogenative Coupling (CDC) Reaction.  
PG - 3283-5  
LID - 10.1021/acs.orglett.5b01479 [doi]  
AB - 2-Perfluoroalkylated indoles were efficiently synthesized via a one-pot cascade Michael-type addition/palladium-catalyzed intramolecular cross-dehydrogenative coupling (CDC) process, using molecular oxygen as the sole oxidant at 100 degrees C in DMSO. This process allows atom economical assembly of indole rings from inexpensive and readily available anilines and methyl perfluoroalk-2-ynoates and tolerates a broad range of functional groups.  
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 LA - eng  
 PT - Journal Article  
 DEP - 20150619  
 PL - United States  
 TA - Org Lett  
 JT - Organic letters  
 JID - 100890393  
 SB - IM  
 EDAT- 2015/06/20 06:00  
 MHDA- 2015/06/20 06:00  
 CRDT- 2015/06/20 06:00  
 PHST- 2015/06/19 [aheadofprint]  
 AID - 10.1021/acs.orglett.5b01479 [doi]  
 PST - ppublish  
 SO - Org Lett. 2015 Jul 2;17(13):3283-5. doi: 10.1021/acs.orglett.5b01479. Epub 2015  
 Jun 19.  
  
 PMID- 26214056  
 OWN - NLM  
 STAT- Publisher  
 DA - 20150727  
 LR - 20150728  
 IS - 1463-9084 (Electronic)  
 IS - 1463-9076 (Linking)  
 DP - 2015 Jul 27  
 TI - Mechanistic details of energy transfer and soft landing in ala-H collisions with  
 a F-SAM surface.  
 AB - Previous chemical dynamics simulations (Phys. Chem. Chem. Phys., 2014, 16,  
 23769-23778) were analyzed to delineate atomistic details for collision of



N-protonated dialanine (ala2-H<sup>+</sup>) with a C8 perfluorinated self-assembled monolayer (F-SAM) surface. Initial collision energies  $E_i$  of 5-70 eV and incident angles  $\theta_{\text{tai}}$  of 0 degrees and 45 degrees, with the surface normal, were considered. Four trajectory types were identified: (1) direct scattering; (2) temporary sticking/physisorption on top of the surface; (3) temporary penetration of the surface with additional physisorption on the surface; and (4) trapping on/in the surface, by physisorption or surface penetration, when the trajectory is terminated. Direct scattering increases from 12 to 100% as  $E_i$  is increased from 5 to 70 eV. For the direct scattering at 70 eV, at least one ala2-H<sup>+</sup> heavy atom penetrated the surface for all of the trajectories. For approximately 33% of the trajectories all eleven of the ala2-H<sup>+</sup> heavy atoms penetrated the F-SAM at the time of deepest penetration. The importance of trapping decreased with increase in  $E_i$ , decreasing from 84 to 0% with  $E_i$  increase from 5 to 70 eV at  $\theta_{\text{tai}} = 0$  degrees. Somewhat surprisingly, the collisional energy transfers to the F-SAM surface and ala2-H<sup>+</sup> are overall insensitive to the trajectory type. The energy transfer to ala2-H<sup>+</sup> is primarily to vibration, with the transfer to rotation approximately 10% or less. Adsorption and then trapping of ala2-H<sup>+</sup> is primarily a multi-step process, and the following five trapping mechanisms were identified: (i) physisorption-penetration-physisorption (phys-pen-phys); (ii) penetration-physisorption-penetration (pen-phys-pen); (iii) penetration-physisorption (pen-phys); (iv) physisorption-penetration (phys-pen); and (v) only physisorption (phys). For  $E_i = 5$  eV, the pen-phys-pen, pen-phys, phys-pen, and phys trapping mechanisms have similar probabilities. For 13.5 eV, the phys-pen mechanism, important at 5 eV, is unimportant. The radius of gyration of ala2-H<sup>+</sup> was calculated once it is trapped on/in the F-SAM surface and trapping decreases the ion's compactness, in part by breaking hydrogen bonds. The ala2-H<sup>+</sup> + F-SAM simulations are compared with the penetration and trapping dynamics found in previous simulations of projectile + organic surface collisions.

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AU - Kohale SC

FAU - Hase, W L

AU - Hase WL

LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150727

TA - Phys Chem Chem Phys

JT - Physical chemistry chemical physics : PCCP

JID - 100888160

EDAT- 2015/07/28 06:00

MHDA- 2015/07/28 06:00

CRDT- 2015/07/28 06:00

AID - 10.1039/c5cp03214h [doi]

PST - aheadofprint

SO - Phys Chem Chem Phys. 2015 Jul 27.

PMID- 25499722

OWN - NLM

STAT- In-Process

DA - 20150609

LR - 20150614

IS - 1873-1708 (Electronic)

IS - 0890-6238 (Linking)

VI - 54

DP - 2015 Jul

TI - The mammary gland is a sensitive pubertal target in CD-1 and C57Bl/6 mice following perinatal perfluorooctanoic acid (PFOA) exposure.

PG - 26-36

LID - 10.1016/j.reprotox.2014.12.002 [doi]

LID - S0890-6238(14)00313-X [pii]

AB - Perfluorooctanoic acid (PFOA) is a developmental toxicant in mice, with varied strain outcomes depending on dose and period of exposure. The impact of PFOA on female mouse pubertal development at low doses ( $\leq 1$  mg/kg) has yet to be determined. Therefore, female offspring from CD-1 and C57Bl/6 dams exposed to PFOA, creating serum concentrations similar to humans, were examined for pubertal onset, including mammary gland development. Pups demonstrated a shorter PFOA elimination half-life than that reported for adult mice. Prenatal exposure to PFOA caused significant mammary developmental delays in female offspring in both strains. Delays started during puberty and persisted into young adulthood; severity was dose-dependent. Also an evaluation of female serum hormone levels and pubertal timing onset revealed no effects of PFOA compared to controls in either strain. These data suggest that the mammary gland is more sensitive to early low level PFOA exposures compared to other pubertal endpoints, regardless of strain.

CI - Published by Elsevier Inc.

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LA - eng

GR - T32 ES007126/ES/NIEHS NIH HHS/United States

GR - ZIA ES102785-03/Intramural NIH HHS/United States

GR - ZIA ES102785-04/Intramural NIH HHS/United States

PT - Journal Article

PT - Research Support, N.I.H., Extramural

DEP - 20141212

PL - United States

TA - Reprod Toxicol

JT - Reproductive toxicology (Elmsford, N.Y.)

JID - 8803591

SB - IM

PMC - PMC4464984

MID - NIHMS648688

OID - NLM: NIHMS648688 [Available on 07/01/16]

OID - NLM: PMC4464984 [Available on 07/01/16]

OTO - NOTNLM

OT - C57Bl/6

OT - CD-1

OT - Estrous cycle

OT - Mammary gland

OT - Perfluorooctanoic acid

OT - Puberty

OT - Vaginal opening

EDAT- 2014/12/17 06:00

MHDA- 2014/12/17 06:00

CRDT- 2014/12/16 06:00

PMCR- 2016/07/01 00:00  
PHST- 2014/08/07 [received]  
PHST- 2014/11/26 [revised]  
PHST- 2014/12/03 [accepted]  
PHST- 2014/12/12 [aheadofprint]  
AID - S0890-6238(14)00313-X [pii]  
AID - 10.1016/j.reprotox.2014.12.002 [doi]  
PST - ppublish  
SO - Reprod Toxicol. 2015 Jul;54:26-36. doi: 10.1016/j.reprotox.2014.12.002. Epub 2014 Dec 12.

PMID- 25828416  
OWN - NLM  
STAT- In-Process  
DA - 20150508  
IS - 1879-1026 (Electronic)  
IS - 0048-9697 (Linking)  
VI - 521-522  
DP - 2015 Jul 15  
TI - Elevated levels of perfluoroalkyl substances in estuarine sediments of Charleston, SC.  
PG - 79-89  
LID - 10.1016/j.scitotenv.2015.03.078 [doi]  
LID - S0048-9697(15)00353-8 [pii]  
AB - Urban areas are sources of perfluoroalkyl substances (PFASs) in the environment, although little is known about specific point sources and distribution of PFASs. Sentinel species, like bottlenose dolphins, are important indicators of environmental perturbations. The high PFAS levels found in dolphins inhabiting Charleston, South Carolina prompted investigation of these chemicals in this area. This study provides further evidence on the extent of contamination and potential sources of PFASs. In this study, concentrations of 11 PFASs measured in estuarine sediments collected in 2012 from the Charleston Harbor and the Ashley and Cooper Rivers (n=36) in South Carolina revealed higher levels than those reported in any other U.S. urban areas. Detectable levels were found in all sample locations with mean total PFAS concentrations of 3.79ngg(-1) (range 0.22 to 19.2ngg(-1) d.w.). Dominant compounds were perfluorooctane sulfonate (PFOS) (mean 1.52ngg(-1); range 0.09-7.37ngg(-1) d.w.), followed by perfluorodecanoate (PFDA) (mean 0.83ngg(-1); range 0.06-4.76ngg(-1) d.w.) and perfluorooctanoate (PFOA) (mean 0.42ngg(-1); range 0.02-2.52ngg(-1) d.w.). PFOS levels in sediments at 19 of 36 sites (representing 52% of the study area) exceeded the published global median PFOS sediment concentration of 0.54ngg(-1).  
CI - Published by Elsevier B.V.  
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LA - eng  
PT - Journal Article  
PT - Research Support, Non-U.S. Gov't  
DEP - 20150328  
PL - Netherlands  
TA - Sci Total Environ  
JT - The Science of the total environment  
JID - 0330500  
SB - IM  
OTO - NOTNLM  
OT - Charleston Harbor  
OT - Perfluoroalkyl substances (PFASs)  
OT - Sediments  
EDAT- 2015/04/02 06:00

MHDA- 2015/04/02 06:00  
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 PHST- 2015/03/19 [revised]  
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 PHST- 2015/03/28 [aheadofprint]  
 AID - S0048-9697(15)00353-8 [pii]  
 AID - 10.1016/j.scitotenv.2015.03.078 [doi]  
 PST - ppublish  
 SO - Sci Total Environ. 2015 Jul 15;521-522:79-89. doi:  
 10.1016/j.scitotenv.2015.03.078. Epub 2015 Mar 28.

PMID- 25817761  
 OWN - NLM  
 STAT- In-Process  
 DA - 20150420  
 IS - 1879-1026 (Electronic)  
 IS - 0048-9697 (Linking)  
 VI - 520  
 DP - 2015 Jul 1  
 TI - Emission factor estimation of ca. 160 emerging organic microcontaminants by  
 inverse modeling in a Mediterranean river basin (Llobregat, NE Spain).  
 PG - 241-52  
 LID - 10.1016/j.scitotenv.2015.03.055 [doi]  
 LID - S0048-9697(15)00330-7 [pii]  
 AB - Starting from measured river concentrations, emission factors of 158 organic  
 compounds out of 199 analyzed belonging to different groups of priority and  
 emerging contaminants [pesticides (25), pharmaceuticals and hormones (81),  
 perfluoroalkyl substances (PFASs) (18), industrial compounds (12), drugs of abuse  
 (8) and personal care products (14)] have been estimated by inverse modeling. The  
 Llobregat river was taken as case study representative of Mediterranean rivers.  
 Industrial compounds and pharmaceuticals are the dominant groups (range of 10(4)  
 mg.1000 inhab(-1).d(-1)). Personal care products, pesticides, PFASs and illegal  
 drugs showed a load approximately one order of magnitude smaller. Considered on a  
 single compound basis industrial compounds still dominate (range of ca. 10(3)  
 mg.1000 inhab(-1).d(-1)) over other classes. Generally, the results are within  
 the range when compared to previously published estimations for other river  
 basins. River attenuation expressed as the percentage fraction of  
 microcontaminants eliminated was quantified. On average they were around 60-70%  
 of the amount discharged for all classes, except for PFASs, that are poorly  
 eliminated (ca. 20% on average). Uncertainties associated with the calculated  
 emissions have been estimated by Monte-Carlo methods (15,000 runs) and typically  
 show coefficients of variation of ca. 120%. Sensitivities associated with the  
 various variables involved in the calculations (river discharge, river length,  
 concentration, elimination constant, hydraulic travel time and river velocity)  
 have been assessed as well. For the intervals chosen for the different variables,  
 all show sensitivities exceeding unity (1.14 to 3.43), tending to amplify the  
 variation of the emission. River velocity and basin length showed the highest

sensitivity value. Even considering the limitations of the approach used, inverse modeling can provide a useful tool for management purposes facilitating the quantification of release rates of chemicals into the aquatic environment.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150325

PL - Netherlands

TA - Sci Total Environ

JT - The Science of the total environment

JID - 0330500

SB - IM

OTO - NOTNLM

OT - Emission factors

OT - Inverse modeling

OT - Llobregat river

OT - Organic micropollutants

OT - Sensitivity

OT - Uncertainty analysis  
 EDAT- 2015/03/31 06:00  
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 AID - S0048-9697(15)00330-7 [pii]  
 AID - 10.1016/j.scitotenv.2015.03.055 [doi]  
 PST - ppublish  
 SO - Sci Total Environ. 2015 Jul 1;520:241-52. doi: 10.1016/j.scitotenv.2015.03.055.  
 Epub 2015 Mar 25.  
  
 PMID- 25882424  
 OWN - NLM  
 STAT- In-Process  
 DA - 20150417  
 IS - 1873-3573 (Electronic)  
 IS - 0039-9140 (Linking)  
 VI - 139  
 DP - 2015 Jul 1  
 TI - Vortex-assisted surfactant-enhanced emulsification liquid-liquid microextraction  
 for the determination of carbamates in juices by micellar electrokinetic  
 chromatography tandem mass spectrometry.  
 PG - 174-80  
 LID - 10.1016/j.talanta.2015.02.057 [doi]  
 LID - S0039-9140(15)00140-X [pii]  
 AB - A new method based on vortex-assisted surfactant-enhanced-emulsification  
 liquid-liquid microextraction has been developed for the extraction of carbamate  
 pesticides in juice samples prior to their determination by micellar  
 electrokinetic chromatography coupled to tandem mass spectrometry. This sample  
 treatment allowed the satisfactory extraction and the extract clean-up of 25  
 carbamates from different fruit and vegetal juices (banana, tomato, and peach).  
 In this study, the addition of ammonium perfluorooctanoate in the aqueous sample  
 in combination with vortex agitation, provided very clean extracts with short  
 extraction times. Under optimized conditions, recoveries of the proposed method  
 for these pesticides from fortified juice samples ranged from 81% to 104%, with  
 relative standard deviations lower than 15%. Limits of quantification were  
 between 2.3microgkg(-)(1) and 4.7microgkg(-)(1), showing the high sensitivity of  
 this fast and simple method.  
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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150309

PL - Netherlands

TA - Talanta

JT - Talanta

JID - 2984816R

SB - IM

OTO - NOTNLM

OT - Carbamates

OT - Juice

OT - Micellar electrokinetic chromatography

OT - Tandem mass spectrometry

OT - Vortex-assisted surfactant-enhanced-emulsification liquid-liquid microextraction

EDAT- 2015/04/18 06:00

MHDA- 2015/04/18 06:00

CRDT- 2015/04/18 06:00

PHST- 2014/11/28 [received]

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AID - S0039-9140(15)00140-X [pii]

AID - 10.1016/j.talanta.2015.02.057 [doi]

PST - ppublish

SO - Talanta. 2015 Jul 1;139:174-80. doi: 10.1016/j.talanta.2015.02.057. Epub 2015 Mar 9.

PMID- 26142696

OWN - NLM

STAT- Publisher

DA - 20150815

LR - 20150815

IS - 1879-3177 (Electronic)

IS - 0887-2333 (Linking)

VI - 29

IP - 7

DP - 2015 Jul 2

TI - In vitro evaluation of the cytotoxicity and modulation of mechanisms associated with inflammation induced by perfluorooctanesulfonate and perfluorooctanoic acid in human colon myofibroblasts CCD-18Co.

PG - 1683-1691

LID - S0887-2333(15)00162-9 [pii]

LID - 10.1016/j.tiv.2015.07.001 [doi]

AB - Perfluorooctanesulfonate (PFOS) and perfluorooctanoic acid (PFOA) are the most notable members of an emerging class of persistent organic pollutants (POPs), poly- and perfluoroalkyl acids (PFASs). In this study, the CCD-18Co myofibroblasts were selected as a cell model to investigate the cytotoxic effects of PFOS and PFOA. The aim was to perform an in vitro evaluation of the ability of these compounds to induce cytotoxicity and modulate mechanisms associated with inflammation as measured by (i) colon fibroblasts viability, (ii) colon fibroblasts proliferation, and (iii) IL-6 production. The data provided in this study suggest that PFOS and PFOA can have cytotoxic potential and modulate processes associated with intestinal inflammation such as myofibroblasts proliferation and IL-6 production at concentrations similar to those detected in vivo. Our results also highlight the influence of culture serum concentration in cytotoxic in vitro studies, which should be considered in future toxicity studies involving PFOS and PFOA. The results contribute to a better knowledge of the effects of PFOS and PFOA in human cells, a phenomenon still not fully examined.

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LA - ENG

PT - JOURNAL ARTICLE

DEP - 20150702

TA - Toxicol In Vitro

JT - Toxicology in vitro : an international journal published in association with BIBRA

JID - 8712158

OTO - NOTNLM

OT - Inflammation

OT - Myofibroblasts CCD18-Co

OT - Perfluorooctanesulfonate

OT - Perfluorooctanoic acid  
 OT - Polyfluoroalkyl and perfluoroalkyl acids  
 EDAT- 2015/07/06 06:00  
 MHDA- 2015/07/06 06:00  
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 AID - S0887-2333(15)00162-9 [pii]  
 AID - 10.1016/j.tiv.2015.07.001 [doi]  
 PST - aheadofprint  
 SO - Toxicol In Vitro. 2015 Jul 2;29(7):1683-1691. doi: 10.1016/j.tiv.2015.07.001.  
  
 PMID- 25868421  
 OWN - NLM  
 STAT- MEDLINE  
 DA - 20150613  
 DCOM- 20150817  
 IS - 1879-3185 (Electronic)  
 IS - 0300-483X (Linking)  
 VI - 333  
 DP - 2015 Jul 3  
 TI - Perfluorooctanoic acid (PFOA) affects distinct molecular signalling pathways in human primary hepatocytes.  
 PG - 53-62  
 LID - 10.1016/j.tox.2015.04.004 [doi]  
 LID - S0300-483X(15)00075-X [pii]  
 AB - Perfluorooctanoic acid (PFOA) was shown to damage the liver of rodents and to impair embryonic development. At the molecular level, the hepatotoxic effects were attributed to the PFOA-mediated activation of peroxisome proliferator-activated receptor alpha (PPARalpha). In general, PPARalpha-dependent effects are less pronounced in humans than in rodents, and the hazard potential of PFOA for humans is controversially discussed. To analyse the effects of PFOA in human hepatocytes, a microarray analysis was conducted to screen for PFOA-mediated alterations in the transcriptome of human primary hepatocytes. A subsequent network analysis revealed that PFOA had an impact on several signalling pathways in addition to the well-known activation of PPARalpha. The microarray data confirmed earlier findings that PFOA: (i) affects the estrogen receptor ERalpha, (ii) activates the peroxisome proliferator-activated receptor gamma (PPARGgamma), and (iii) inhibits the function of the hepatocyte nuclear factor 4alpha (HNF4alpha) which is an essential factor for liver development and embryogenesis. Finally, as a novel finding, PFOA was shown to stimulate gene expression of the proto-oncogenes c-Jun and c-Fos. This was confirmed by using the HepG2 cell line as a model for human hepatocytes. PFOA stimulated cellular proliferation and the metabolic activity of the cells, and upregulated the expression of various cyclins which have a central function in the regulation of cell cycle control. Functional studies, however, indicated that PFOA had no impact on c-Jun and c-Fos phosphorylation and on

AP-1-dependent gene transcription, thus demonstrating that PFOA-induced proliferation occurs largely independent of c-Jun and c-Fos.

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LA - eng

PT - Journal Article

PT - Research Support, Non-U.S. Gov't

DEP - 20150411

PL - Ireland

TA - Toxicology

JT - Toxicology

JID - 0361055

RN - 0 (Caprylates)

RN - 0 (Cyclins)

RN - 0 (Estrogen Receptor alpha)

RN - 0 (Fluorocarbons)

RN - 0 (HNF4A protein, human)

RN - 0 (Hepatocyte Nuclear Factor 4)

RN - 0 (PPAR alpha)

RN - 0 (PPAR gamma)

RN - 0 (Proto-Oncogene Proteins c-fos)

RN - 0 (Proto-Oncogene Proteins c-jun)

RN - 0 (Transcription Factor AP-1)

RN - 0 (estrogen receptor alpha, human)

RN - 335-67-1 (perfluorooctanoic acid)

SB - IM  
 MH - Caprylates/\*toxicity  
 MH - Cell Cycle/drug effects  
 MH - Cell Proliferation/drug effects  
 MH - Cyclins/genetics/metabolism  
 MH - Dose-Response Relationship, Drug  
 MH - Drug-Induced Liver Injury/\*etiology/genetics/metabolism/pathology  
 MH - Estrogen Receptor alpha/agonists/genetics/metabolism  
 MH - Fluorocarbons/\*toxicity  
 MH - Gene Expression Profiling/methods  
 MH - Gene Expression Regulation  
 MH - Gene Regulatory Networks  
 MH - Hep G2 Cells  
 MH - Hepatocyte Nuclear Factor 4/antagonists & inhibitors/genetics/metabolism  
 MH - Hepatocytes/\*drug effects/metabolism/pathology  
 MH - Humans  
 MH - Oligonucleotide Array Sequence Analysis  
 MH - PPAR alpha/agonists/genetics/metabolism  
 MH - PPAR gamma/agonists/genetics/metabolism  
 MH - Primary Cell Culture  
 MH - Proto-Oncogene Proteins c-fos/genetics/metabolism  
 MH - Proto-Oncogene Proteins c-jun/genetics/metabolism  
 MH - Signal Transduction/\*drug effects  
 MH - Time Factors  
 MH - Transcription Factor AP-1/genetics/metabolism  
 MH - Transcriptome  
 OTO - NOTNLM  
 OT - Cell cycle regulation  
 OT - Hepatocyte  
 OT - PFOA  
 OT - Transcriptomics  
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